



Dynamics and Thermodynamics of Simple Two-Phase Reacting Mixtures for Application to Explosive Initiation Modeling

by John Starkenberg

ARL-TR-2161

March 2000

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ARL-TR-2161

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Abstract

The front-tracking "hydrocode" *FRONTIER* limits finite-difference solution of the dynamic continuum mechanics equations to regions bounded by tracked fronts (shock waves, contact discontinuities, and gradient discontinuities) and uses local solutions of the Riemann problem to advance the positions of these fronts. This solution method places stringent requirements on the availability of thermodynamics information. With the addition of an appropriate reacting mixture model, the code can be applied to solid explosive initiation problems. The required thermodynamic functions are more difficult to obtain for reacting mixtures even though the equations of state for each of the phases present are known. We have developed a mixture model based on assumptions of mechanical equilibrium and thermal isolation that can be used independent of the choice of equations of state for the phases, and we have derived expressions for the necessary thermodynamic functions.

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1. Background

We are working to adapt *FRONTIER*, a front-tracking "hydrocode" developed at the State University of New York at Stony Brook (Glimm et al. 1981, 1985; Grove 1989, 1993), for application to solid explosive initiation problems. The principal elements required to treat such problems numerically are a continuum mechanics model (including appropriate treatment of boundary conditions) and a reacting mixture model. The former is represented by a system of dynamic partial differential equations and the latter by a system of algebraic equations (augmented, in some cases, by additional dynamic equations). The forms of these models depend on the assumptions used.

FRONTIER is unique in that it limits finite-difference solution of the dynamic continuum mechanics equations to regions bounded by tracked fronts. These may include shock waves, contact discontinuities (i.e., material interfaces and slip lines), and gradient discontinuities (e.g., boundaries between simple and complex wave regions). The front-tracking method superimposes grids for these fronts on the computational region. For an n -dimensional computational region, the grids are of dimension $n-1$. The method uses local solutions of the Riemann problem coupled to the interior region solution to advance the positions of tracked shock waves and contact discontinuities. There results a description of the flow that retains the discontinuous character of the fronts. This solution method places stringent requirements on the availability of thermodynamic information. In addition to the incomplete equation of state for pressure required by all hydrocodes, the Riemann solvers require expressions for the acoustic impedance, sound speed and adiabatic exponent, and the Grüneisen function, as well as adiabats and Hugoniot. While these are readily developed from most equations of state, they are more difficult to obtain for reacting mixtures.

In order to avoid the need to completely rework *FRONTIER*'s coding for solution of material dynamics, we are interested in mixture models that, insofar as possible, allow retention of the gas dynamics conservation equations for diffusionless flow. The extent to which this objective may be achieved depends on the physical assumptions that we wish to apply. Usually, the requirement can be met, although additional dynamic equations may arise. It is generally necessary to add a dynamic equation representing reaction progress.

Several modeling approaches applicable to mixtures of discrete phases have been reported in the literature, and some of these are reviewed and amplified here. The set of physical assumptions that appears to best apply to explosive initiation includes mechanical equilibrium and thermal isolation between reactant and product phases. While the thermal isolation condition can be implemented as an added dynamic equation, representing partitioning of the energy conservation equation between the phases, including it in the mixture model is more consistent with our desire to retain the original form of the conservation equations. We have developed a model along these lines that can be used independently of the choice of equations of state for the phases and have derived expressions for the necessary thermodynamic functions.

2. Mixture and Phase Variables

Consider a Lagrangian control volume, ΔV , containing a mixture of two phases having mass ΔM . Phase variables are denoted by subscripts r and p (anticipating but not limited to reactants and products), while mixture variables are unsubscripted. The mass of the mixture is equal to the sum of the phase masses:

$$\Delta M = \Delta M_r + \Delta M_p .$$

Dividing by ΔM gives

$$\frac{\Delta M_r}{\Delta M} + \frac{\Delta M_p}{\Delta M} = 1 .$$

Mass fractions for each phase can be defined as

$$\lambda_r = \lim_{\Delta M \rightarrow 0} \frac{\Delta M_r}{\Delta M} ,$$

and

$$\lambda_p = \lim_{\Delta M \rightarrow 0} \frac{\Delta M_p}{\Delta M} ,$$

so that

$$\lambda_r + \lambda_p = 1 .$$

In light of this simple relation, a single mass fraction variable, λ , may be chosen so that

$$\lambda_r = 1 - \lambda$$

and

$$\lambda_p = \lambda .$$

Similarly, volume fractions are defined as

$$\eta_r = 1 - \eta = \lim_{\Delta V \rightarrow 0} \frac{\Delta V_r}{\Delta V} ,$$

and

$$\eta_p = \eta = \lim_{\Delta V \rightarrow 0} \frac{\Delta V_p}{\Delta V} .$$

The mixture and phase specific volumes are defined as

$$v = \lim_{\Delta M \rightarrow 0} \frac{\Delta V}{\Delta M} ,$$

$$v_r = \lim_{\Delta M \rightarrow 0} \frac{\Delta V_r}{\Delta M_r},$$

and

$$v_p = \lim_{\Delta M \rightarrow 0} \frac{\Delta V_p}{\Delta M_p}.$$

Thus,

$$(1-\lambda) v_r = (1-\eta) v,$$

and

$$\lambda v_p = \eta v.$$

The mixture is said to be saturated if its volume equals the sum of the phase volumes:

$$\Delta V = \Delta V_r + \Delta V_p.$$

This assumption is most appropriate when one of the phases is gaseous, as is generally the case for detonation. Dividing by ΔM gives

$$\frac{\Delta V}{\Delta M} = \frac{\Delta V_r}{\Delta M_r} \frac{\Delta M_r}{\Delta M} + \frac{\Delta V_p}{\Delta M_p} \frac{\Delta M_p}{\Delta M},$$

so that

$$v = (1-\lambda) v_r + \lambda v_p.$$

Similar considerations yield saturation conditions for the mixture and phase specific internal energies and specific entropies:

$$e = (1 - \lambda) e_r + \lambda e_p,$$

and

$$s = (1 - \lambda) s_r + \lambda s_p.$$

3. Conservation Equations

It is assumed that the values of some of the variables required to describe the mixture are available from integration of continuum mechanics conservation equations. Since the material strengths of explosives are generally modest and the pressures associated with their initiation high, the equations of gas dynamics can be used:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p = 0,$$

and

$$\frac{\partial}{\partial t} (\rho e_T) + \nabla \cdot (\rho e_T \mathbf{u}) + \nabla \cdot (p \mathbf{u}) = 0,$$

where t is time, ρ is the density, \mathbf{u} is the particle velocity vector, p is the pressure, e_T is the total specific energy,

$$e_T = e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u},$$

and e is the specific internal energy. This system is generally closed by obtaining pressure as a function of density (or specific volume, $v = 1/\rho$) and specific internal energy from an incomplete equation of state:

$$p = p(v, e) .$$

In order to apply the gas dynamics equations to a discrete mixture, an incomplete equation of state yielding a single pressure for the mixture is required. This pressure will, additionally, depend on a reaction progress variable:

$$p = p(v, e, \lambda) .$$

Further, the phase pressures should equal the mixture pressure. Otherwise, the momentum and energy conservation equations must be split between the phases. Splitting is also required if the flow is not diffusionless (i.e., the same particle velocity should apply to both phases).

Where the mixture is reacting, the reaction progress must be computed, and the energy liberated during the reaction must be accounted for. Additional variables and equations are required for these purposes. However, the conservation equations in the form shown apply as long as single pressures and particle velocities are maintained. The reaction rate equation is

$$\frac{\partial}{\partial t}(\rho \lambda) + \nabla \cdot (\rho \lambda \mathbf{u}) = \rho \dot{\lambda}(\lambda, p, \dots) ,$$

where the reaction rate is a known function of state and history variables obtained from one of a number of available models. The equation arises as a consequence of conservation of mass and must be integrated along with the other conservation equations.

The chemical energy released in the reaction process must also be accounted for. This could be done by modifying the energy conservation equation such that

$$\frac{\partial}{\partial t}(\rho e_T) + \nabla \cdot (\rho e_T \mathbf{u}) + \nabla \cdot (p \mathbf{u}) = -\rho \Delta h_D \dot{\lambda}(\lambda, p, \dots),$$

where Δh_D is the (negative) heat of detonation. However, this is inconsistent with our desire to retain the original conservation equations and it can be accomplished more simply by regarding the reactant phase specific internal energy as composed of a thermal component and a potential component equal to the absolute value of the heat of detonation:

$$e_r = e_{r,thermal} - \Delta h_D.$$

The reactant phase equation of state (as developed in Appendix A) applies only to the thermal component,

$$e_{r,thermal} = e_r + \Delta h_D,$$

and the reactant phase equation of state for pressure may be expressed

$$p_r = p_r(v_r, e_r + \Delta h_D).$$

In practice, the heat of detonation is often included in the equation of state.

4. Mixture Equations of State

4.1 General. Returning to our Lagrangian control volume, we may write the complete equation of state for the mixture:

$$\Delta E = E(\Delta V, \Delta S, \Delta M_r, \Delta M_p),$$

where ΔS is the entropy. Because of the homogeneous first-order nature of such equations, dividing by ΔM gives

$$\frac{\Delta E}{\Delta M} = E\left(\frac{\Delta V}{\Delta M}, \frac{\Delta S}{\Delta M}, \frac{\Delta M_r}{\Delta M}, \frac{\Delta M_p}{\Delta M}\right).$$

Thus, in the limit as ΔM vanishes,

$$e = E(v, s, \lambda_r, \lambda_p) = e(v, s, \lambda) .$$

Incomplete equations of state are obtained by differentiating:

$$p(v, s, \lambda) = - \left(\frac{\partial e}{\partial v} \right)_{s, \lambda}$$

and

$$T(v, s, \lambda) = \left(\frac{\partial e}{\partial s} \right)_{v, \lambda} ,$$

where T is the temperature. Additionally,

$$\mu(v, s, \lambda) = \left(\frac{\partial e}{\partial \lambda} \right)_{v, s}$$

defines the normalized chemical potential. By solving the complete equation of state for the specific entropy,

$$s = s(v, e, \lambda) ,$$

and substituting into the incomplete equation of state for pressure, we obtain the form required for solution of the gas dynamics conservation equations (i.e., with v , e , and λ as the three independent variables):

$$p = p(v, e, \lambda) .$$

However, the complete equation of state is generally unavailable. Rather, incomplete equations of state for each phase giving pressure as a function of specific volume and internal energy are known:

$$p_r = p_r(v_r, e_r + \Delta h_D) ,$$

and

$$p_p = p_p(v_p, e_p) .$$

In order to establish an equation of state for the mixture, we may combine these with the volume and energy saturation conditions:

$$v = (1 - \lambda) v_r + \lambda v_p$$

and

$$e = (1 - \lambda) e_r + \lambda e_p .$$

This is a system of four equations in nine variables (v , e , λ , v_r , e_r , p_r , v_p , e_p , and p_p), not including the pressure. Thus, two additional equations are required to produce a solution for the pressure as a function of three independent variables.

4.2 Equilibrium Assumptions. The number of independent variables can be reduced by invoking assumptions of physical equilibrium. The most common of these, the assumption of mechanical equilibrium (Mader 1979; Johnson, Tang, and Forest 1985; Starkenberg 1989), is required to retain the simplified form of the conservation equations. It implies that the phases are at equal pressures and is achieved by a relatively rapid wave propagation mechanism. Thus,

$$p_r(v_r, e_r + \Delta h_D) = p_p(v_p, e_p) .$$

Another assumption that has been used (Mader 1979) is that of thermal equilibrium. In this case, the phases are at equal temperatures, presumably by virtue of significantly slower conductive processes, and incomplete equations of state for the phase temperatures are required:

$$T_r(v_r, e_r + \Delta h_D) = T_p(v_p, e_p) .$$

Thus, with both mechanical and thermal equilibrium, the mixture equation of state may be expressed as

$$v_r = v_r(v, e, \lambda),$$

$$v_p = v_p(v, e, \lambda),$$

$$e_r = e_r(v, e, \lambda),$$

$$e_p = e_p(v, e, \lambda),$$

$$p = p(v, e, \lambda),$$

$$T = T(v, e, \lambda).$$

This formulation has the desired set of independent variables. However, because thermal equilibrium can be achieved only through physical processes that generally act slowly compared to pressure equilibration and are consequently physically unrealistic in explosive initiation environments, alternatives to this assumption have been sought.

4.3 Thermal Isolation. The thermal isolation condition, which represents the opposite extreme and appears more realistic than thermal equilibrium, was used in Lagrangian computations by Johnson, Tang, and Forest (1985) and in conjunction with smoothed particle hydrodynamics by Libersky (1993). These approaches were limited to use with a linear- Γ Mie-Grüneisen equation of state for the reactant phase. Here, we shall relax this limitation and generalize the approach for use with any equation of state.

If the mixture is constrained to change its state such that the phases remain thermally isolated, there results an isentropic process for the reactant phase. Thus, the thermal isolation condition may be expressed

$$p_r(v_r, e_r + \Delta h_D) = p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D),$$

or

$$e_r + \Delta h_D = e_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) ,$$

or simply

$$s_r(v_r, e_r + \Delta h_D) = s_{rk} = s_r(v_{rk}, e_{rk} + \Delta h_D) ,$$

where the isentrope functions are known and (v_{rk}, e_{rk}) is a reference state specifying the isentrope. If the material has been shocked, this state is, most conveniently, that existing on the Hugoniot immediately after the most recent shock passage. Otherwise, the initial state may be used. In an Eulerian numerical computation, this state can be advected for use throughout the reactive flow field:

$$\frac{\partial}{\partial t} (\rho v_{rk}) + \nabla \cdot (\rho v_{rk} \mathbf{u}) = 0 ,$$

and

$$\frac{\partial}{\partial t} (\rho e_{rk}) + \nabla \cdot (\rho e_{rk} \mathbf{u}) = 0 .$$

Unfortunately, where artificial viscosity is used to capture shock waves, the accurate determination of shocked states (and, hence, the accurate initialization of the reference state following shock passage) is not generally possible. The front-tracking approach, on the other hand, provides an opportunity to accurately initialize and advect (v_{rk}, e_{rk}) .

4.4 Other Models. Because the iterative processes associated with the foregoing approaches may be time consuming (although convergence should generally be rapid), an alternative approach (Kerley 1992) has been used in the Sandia National Laboratory's CTH code. This is referred to as the "two-state" model. Here, the mixture equation of state is expressed as follows:

$$p(\rho, T, \lambda) = (1 - \lambda) p_r(\rho, T) + \lambda p_p(\rho, T) ,$$

and

$$e(\rho, T, \lambda) = (1 - \lambda) e_r(\rho, T) + \lambda e_p(\rho, T) .$$

Thus, each phase is assumed to have the density and temperature of the mixture, and the mixture pressure is a weighted average of the phase pressures and has no physical meaning. Because of the poor physical fidelity associated with these assumptions, we did not consider it to be a desirable candidate for incorporation into *FRONTIER*. The approach has been eliminated for the 1999 release of CTH.

In addition, Baer and Nunziato (1986) have developed a nonequilibrium model with diffusion for CTH based on physical assumptions. Because this model was primarily intended for porous materials, has exhibited difficulties (Menikoff 1996), and requires substantially more complex conservation equations, it was not considered for application in the front-tracking environment.

4.5 Physical Considerations. To this point, our physical assumptions have been driven by the heuristic purpose of retaining the gas dynamics conservation equations. In spite of this, there remains a variety of circumstances under which the assumptions of diffusionless flow in mechanical equilibrium and thermal isolation may be regarded as physically reasonable.

The physical justification for these assumptions begins with the notion that the process of explosive initiation starts at hot spots that are excited by the interaction between a passing shock wave and the heterogeneities in the explosive. Such hot spots have been observed experimentally by von Holle and Tarver (1981). They are distributed on the scale of the heterogeneities and represent a very small fraction of the explosive mass. There are assumed to be numerous hot spots in any control volume used to derive equations of motion. The hot spots, which may be idealized as closed regions, are assumed to react thermally and to produce "holes" bounded by closed surfaces. The reaction is assumed to propagate further by a surface burning mechanism akin to that observed for propellants in strand burner experiments, which occurs at uniform pressure. This portion of the reaction process is often referred to as hole burning. As reaction proceeds, the holes join, and, before long, discrete solid particles appear embedded in a gas phase matrix. At this point, the process is called grain burning. The point of transition from hole burning to grain burning depends on the

shape of the holes and the way in which they evolve. This description is applicable to the initiation of condensed energetic material by a process referred to as shock-to-detonation transition. Porous materials exhibit a more complex initiation process referred to as deflagration-to-detonation transition in which diffusion may play a role.

The assumption of diffusionless flow is easiest to defend within the surface-burning context. During the early stages of reaction, the gas is entrapped within the solid phase and may not diffuse. During the late stages of reaction, high drag forces acting on the remaining solid resist any tendency toward diffusion. But, most importantly, since burning is assumed to occur at closed surfaces throughout the process, the net momentum of the products relative to the reactants tends to vanish. Mechanical equilibrium is more difficult to justify. It rests on the assumption that burning occurs as observed on a macroscopic scale for propellants. Assuming thermal equilibrium appears unjustified for the rapid processes associated with initiation of detonation. Thermal isolation lies at the opposite extreme and is valid when the reaction process is sufficiently rapid.

Wackerle and Anderson (1984) have shown that simplified representations of the surface reaction rate and the equilibrium state may be inconsistent with the assumed reaction topology. However, in the context of an explosive initiation model, all of this may be moot. Such a model is completed by specifying a reaction rate function containing constants that are calibrated with respect to certain explosive sensitivity experiments. Thus, some excellent results are achieved with highly questionable "equilibrium" assumptions. No advantage to more complex models has yet been exhibited.

5. A Discrete Mixture Equation of State

5.1 General. The equations governing the mixture in mechanical equilibrium and thermal isolation are

$$v = (1-\lambda) v_r + \lambda v_p,$$

$$e = (1-\lambda) e_r + \lambda e_p,$$

$$p = p_r(v_r, e_r + \Delta h_D),$$

$$p = p_p(v_p, e_p),$$

and

$$p = p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D),$$

or

$$e_r + \Delta h_D = e_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D).$$

This constitutes an incomplete equation of state for the mixture pressure and phase states that includes the reactant reference state as an independent variable:

$$v_r = v_r(v, e, \lambda; v_{rk}, e_{rk} + \Delta h_D),$$

$$v_p = v_p(v, e, \lambda; v_{rk}, e_{rk} + \Delta h_D),$$

$$e_r = e_r(v, e, \lambda; v_{rk}, e_{rk} + \Delta h_D),$$

$$e_p = e_p(v, e, \lambda; v_{rk}, e_{rk} + \Delta h_D),$$

and

$$p = p(v, e, \lambda; v_{rk}, e_{rk} + \Delta h_D).$$

5.2 Mixture-Equation Solutions. Because closed form solutions to the system of equations describing the mixture cannot generally be found, it is necessary to obtain solutions using iterative approaches. It is assumed that initial estimates for the values of the unknown variables are available:

$$v_r^{(0)}, v_p^{(0)}, e_r^{(0)}, e_p^{(0)}.$$

If these are known to sufficient accuracy, successively more accurate solutions, given by

$$v_r^{(k+1)} = v_r^{(k)} + \delta v_r^{(k)},$$

$$v_p^{(k+1)} = v_p^{(k)} + \delta v_p^{(k)},$$

$$e_r^{(k+1)} = e_r^{(k)} + \delta e_r^{(k)},$$

and

$$e_p^{(k+1)} = e_p^{(k)} + \delta e_p^{(k)},$$

may be obtained using Newton's method. Other methods may be used until accuracy sufficient for convergence of Newton's method has been achieved. Substituting these solutions into the original equations (eliminating the superscripts for clarity) yields the variational equations,

$$(1-\lambda)\delta v_r + \lambda\delta v_p = v - (1-\lambda)v_r - \lambda v_p,$$

$$(1-\lambda)\delta e_r + \lambda\delta e_p = e - (1-\lambda)e_r - \lambda e_p,$$

$$\left(\frac{\partial p_r}{\partial v_r}\right)_{e_r} \delta v_r + \left(\frac{\partial p_r}{\partial e_r}\right)_{v_r} \delta e_r - \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} \delta v_p - \left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} \delta e_p = p_p(v_p, e_p) - p_r(v_r, e_r + \Delta h_D),$$

and

$$p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) \delta v_r + \delta e_r = e_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) - (e_r + \Delta h_D).$$

These equations are then solved for δv_r , δv_p , δe_r and δe_p , and the solution is updated. The procedure is repeated until the desired accuracy is achieved.

In hydrocode applications, ρ_{Sr} and e_{Sr} can be evaluated by calls to appropriate equation-of-state subroutines. The isentrope reference state, on the other hand, is an integrated variable of the flow and must be included in the call to the mixture-equation-of-state routine.

5.3 Mixture Derivatives. Expressions for the derivatives of the independent state variables with respect to the dependent state variables are developed in Appendix B. Derivatives of the pressure are

$$\left(\frac{\partial p}{\partial v} \right)_{e,\lambda} = \frac{i_r^2}{I^2} \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p}$$

and

$$\left(\frac{\partial p}{\partial e} \right)_{v,\lambda} = \frac{i_r^2}{I^2} \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p},$$

where

$$I^2 = \lambda i_r^2 + (1 - \lambda) i_p^2$$

and i_r^2 and i_p^2 are the squares of the acoustic impedances of the phases, defined as

$$i_m^2 = - \left(\frac{\partial p_m}{\partial v_m} \right)_{s_m} = p \left(\frac{\partial p_m}{\partial e_m} \right)_{v_m} - \left(\frac{\partial p_m}{\partial v_m} \right)_{e_m} \quad m = r, p.$$

With these derivatives in hand, we may proceed to relate thermodynamic functions of the mixture to their phase counterparts.

5.4 Sound Speed and Related Functions. The square of the acoustic impedance of the mixture may be written

$$j^2 = -\left(\frac{\partial p}{\partial v}\right)_{s,\lambda} = p\left(\frac{\partial p}{\partial e}\right)_{v,\lambda} - \left(\frac{\partial p}{\partial v}\right)_{e,\lambda} = \frac{j_r^2 j_p^2}{j^2}.$$

It varies continuously from that of the reactants to that of the products as the mass fraction varies from 0 to 1, and its reciprocal is subject to a saturation condition:

$$\frac{1}{j^2} = \frac{1-\lambda}{j_r^2} + \frac{\lambda}{j_p^2}.$$

The square of the sound speed may be defined in terms of the square of the acoustic impedance:

$$c^2 = j^2 v^2 = \frac{v^2 c_r^2 c_p^2}{(1-\lambda) v_r^2 c_p^2 + \lambda v_p^2 c_r^2}.$$

The corresponding saturation condition is

$$\left(\frac{v}{c}\right)^2 = (1-\lambda)\left(\frac{v_r}{c_r}\right)^2 + \lambda\left(\frac{v_p}{c_p}\right)^2.$$

Another important function defined in terms of the square of the acoustic impedance is the adiabatic exponent, given by

$$\gamma = \frac{j^2 v}{p} = \frac{v \gamma_r \gamma_p}{(1-\lambda) v_r \gamma_p + \lambda v_p \gamma_r} = \frac{\gamma_r \gamma_p}{(1-\eta) \gamma_p + \eta \gamma_r},$$

with the saturation condition

$$\frac{\gamma}{\gamma} = (1-\lambda)\frac{\gamma_r}{\gamma_r} + \lambda\frac{\gamma_p}{\gamma_p}.$$

5.5 Grüneisen Function. The Grüneisen function of the mixture is

$$\Gamma = v \left(\frac{\partial p}{\partial e} \right)_{v,\lambda} = \frac{j^2 v}{j_p^2 v_p} \Gamma_p = \frac{v}{v_p} \Gamma_p .$$

The continuity of this expression for vanishing λ has not been established.

5.6 Temperature and Specific Heat. In order to determine the thermodynamic temperature of the mixture, we begin by differentiating the saturation condition for the entropy with respect to s :

$$(1-\lambda) \left(\frac{\partial s_r}{\partial s} \right)_{v,\lambda} + \lambda \left(\frac{\partial s_p}{\partial s} \right)_{v,\lambda} = 1 .$$

Noting that the thermal isolation condition implies that s_r is a constant, we find that

$$\left(\frac{\partial s_r}{\partial s} \right)_{v,\lambda} = 0 ,$$

and

$$\left(\frac{\partial s_p}{\partial s} \right)_{v,\lambda} = \frac{1}{\lambda} .$$

Differentiating the saturation condition for the specific volume with respect to s gives

$$(1-\lambda) \left(\frac{\partial v_r}{\partial s} \right)_{v,\lambda} + \lambda \left(\frac{\partial v_p}{\partial s} \right)_{v,\lambda} = 0 .$$

We may write the mechanical equilibrium condition in the form

$$p_r(v_r, s_r) = p_p(v_p, s_p) ,$$

and differentiate with respect to s to obtain

$$i_p^2 \left(\frac{\partial v_p}{\partial s} \right)_{v,\lambda} - i_r^2 \left(\frac{\partial v_r}{\partial s} \right)_{v,\lambda} = \frac{\Gamma_p T_p}{v_p l^2}.$$

Thus,

$$\left(\frac{\partial v_r}{\partial s} \right)_{v,\lambda} = - \frac{\Gamma_p T_p}{v_p l^2},$$

and

$$\left(\frac{\partial v_p}{\partial s} \right)_{v,\lambda} = \frac{1-\lambda}{\lambda} \frac{\Gamma_p T_p}{v_p l^2}.$$

Finally, the temperature is determined from its definition,

$$T = \left(\frac{\partial e}{\partial s} \right)_{v,\lambda},$$

by differentiating the saturation condition for the specific internal energy,

$$e(v, s, \lambda) = (1-\lambda) e_r(v_r, s_r) + \lambda e_p(v_p, s_p).$$

This shows that the mixture temperature is simply equal to the product temperature:

$$T(v, e, \lambda) = T_p[v_p(v, e, \lambda), e_p(v, e, \lambda)].$$

The latter can be computed if an incomplete equation of state for the products giving temperature as a function of specific volume and specific internal energy is available. The continuity of this expression for vanishing λ has not been established.

Similarly, the specific heat at constant volume of the mixture may be determined from its definition,

$$c_v = \left(\frac{\partial e}{\partial T} \right)_{v, \lambda},$$

by differentiating the expressions

$$e(v, T, \lambda) = (1 - \lambda) e_r(v_r, T_r) + \lambda e_p(v_p, T_p),$$

$$v = (1 - \lambda) v_r + \lambda v_p,$$

$$T = T_p,$$

$$p_r(v_r, T_r) = p_p(v_p, T_p),$$

and

$$p_r(v_r, T_r) = p_{Sr}(v_r),$$

with respect to T . This shows that the mixture specific heat is given by

$$c_v = \frac{\lambda I^2 c_{v_p}}{I^2 - (1 - \lambda) c_{v_p} T_p \left(\frac{\Gamma_p}{v_p} \right)^2}.$$

Similarly, the continuity of this expression for vanishing λ has not been established.

5.7 Adiat. The complete equation of state of the mixture may be expressed

$$e = e(v, s, \lambda).$$

Its differential is given by

$$de = Tds - p dv + \mu d\lambda ,$$

and the condition defining the mixture adiabat is

$$de + p dv = Tds + \mu d\lambda = 0 .$$

Thus, changes in entropy along the adiabat are associated with chemical reaction. In the absence of reaction, the adiabat becomes an isentrope.

5.8 Hugoniot. We cannot use the mixture equation of state to determine a Hugoniot for the mixture because the reactant isentrope reference state changes across a shock wave. In this case, we make use of known equations of state and Hugoniots for the phases:

$$p = p_r(v_r, e_r + \Delta h_D) ,$$

$$p = p_{Hr}(v_r; p_u, v_{ru}) ,$$

$$p = p_p(v_p, e_p) ,$$

$$p = p_{Hp}(v_p; p_u, v_{pu}) .$$

And the saturation conditions still apply:

$$v = (1 - \lambda) v_r + \lambda v_p ,$$

$$e = (1 - \lambda) e_r + \lambda e_p .$$

This is a system of six equations in eight variables, and the resulting Hugoniot may be expressed

$$\begin{aligned}
 p &= p_H(v, \lambda; p_u, v_u), \\
 e &= e_H(v, \lambda; p_u, v_u), \\
 v_r &= v_{rH}(v, \lambda; p_u, v_u), \\
 e_r &= e_{rH}(v, \lambda; p_u, v_u), \\
 v_p &= v_{pH}(v, \lambda; p_u, v_u), \\
 e_p &= e_{pH}(v, \lambda; p_u, v_u).
 \end{aligned}$$

Finally, a model for the increase in mass fraction across the shock is required:

$$\lambda = \lambda_u + \Delta\lambda_H(v, e).$$

The assumption that no reaction occurs in a shock wave,

$$\lambda = \lambda_u,$$

is consistent with a finite reaction rate. The reactant isentrope reference state for use downstream of the shock is given by

$$v_{rk} = v_r,$$

$$e_{rk} = e_r.$$

5.9 Limiting Solutions. The determinant of coefficients for the variational equations used to solve the mixture equation of state is the same as that given in Appendix B for computation of the

derivatives of the mixture equation of state. In the case of thermal isolation, a singularity arises associated with the vanishing of this determinant at $\lambda = 0$. In this limit, the reactant state is identical to the mixture state. Special considerations are, then, necessary to determine the product state. The set of equations obtained by differentiating the saturation and thermal isolation conditions while retaining the mechanical equilibrium condition is

$$(1-\lambda) \left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e} + \lambda \left(\frac{\partial v_p}{\partial \lambda} \right)_{v,e} = v_r - v_p ,$$

$$(1-\lambda) \left(\frac{\partial e_r}{\partial \lambda} \right)_{v,e} + \lambda \left(\frac{\partial e_p}{\partial \lambda} \right)_{v,e} = e_r - e_p ,$$

$$p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) - p_p(v_p, e_p) = 0 ,$$

and

$$p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e} + \left(\frac{\partial e_r}{\partial \lambda} \right)_{v,e} = 0 .$$

For vanishing λ , these become

$$\left(\frac{\partial v_r}{\partial \lambda} \right)_{\lambda=0} = v - v_{p0} ,$$

$$\left(\frac{\partial e_r}{\partial \lambda} \right)_{\lambda=0} = e - e_{p0} ,$$

$$p_p(v_{p0}, e_{p0}) = p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) ,$$

and

$$p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial v_r}{\partial \lambda} \right)_{\lambda=0} + \left(\frac{\partial e_r}{\partial \lambda} \right)_{\lambda=0} = 0 .$$

This represents a system of equations in the product variables and the first derivatives of the reactant variables with respect to λ . Substituting the expressions for these derivatives into the thermal isolation condition and coupling with the mechanical equilibrium condition gives the equations

$$p_p(v_{p0}, e_{p0}) = p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D),$$

and

$$p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) (v - v_{p0}) = e_{p0} - e,$$

which can be solved for the product state when $\lambda = 0$.

In order to obtain a solution valid near $\lambda = 0$, derivatives with respect to λ may be used in conjunction with Taylor's series. To obtain first derivatives of the product variables and second derivatives of the reactant variables, the set of equations is differentiated again, noting that

$$-\frac{dp_{Sr}}{dv} = -i_{Sr}^2(v; v_{rk}, e_{rk} + \Delta h_D).$$

This gives

$$(1-\lambda) \left(\frac{\partial^2 v_r}{\partial \lambda^2} \right)_{v,e} + \lambda \left(\frac{\partial^2 v_p}{\partial \lambda^2} \right)_{v,e} = 2 \left[\left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e} - \left(\frac{\partial v_p}{\partial \lambda} \right)_{v,e} \right],$$

$$(1-\lambda) \left(\frac{\partial^2 e_r}{\partial \lambda^2} \right)_{v,e} + \lambda \left(\frac{\partial^2 e_p}{\partial \lambda^2} \right)_{v,e} = 2 \left[\left(\frac{\partial e_r}{\partial \lambda} \right)_{v,e} - \left(\frac{\partial e_p}{\partial \lambda} \right)_{v,e} \right],$$

$$\left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} \left(\frac{\partial v_p}{\partial \lambda} \right)_{v,e} + \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \left(\frac{\partial e_p}{\partial \lambda} \right)_{v,e} = -i_{Sr}^2(v; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e},$$

and

$$p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial^2 v_r}{\partial \lambda^2} \right)_{v,e} + \left(\frac{\partial^2 e_r}{\partial \lambda^2} \right)_{v,e} = i_{Sr}^2(v_r; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e}^2 .$$

For vanishing λ , these become

$$\left(\frac{\partial^2 v_r}{\partial \lambda^2} \right)_{\lambda=0} = 2 \left[(v - v_{p0}) - \left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} \right] ,$$

$$\left(\frac{\partial^2 e_r}{\partial \lambda^2} \right)_{\lambda=0} = 2 \left[(e - e_{p0}) - \left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} \right] ,$$

$$\left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} \left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} + \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} = -i_{Sr}^2(v; v_{rk}, e_{rk} + \Delta h_D) (v - v_{p0}) \equiv p_0(v) ,$$

and

$$p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial^2 v_r}{\partial \lambda^2} \right)_{\lambda=0} + \left(\frac{\partial^2 e_r}{\partial \lambda^2} \right)_{\lambda=0} = -p_0(v) (v - v_{p0}) .$$

Substituting the expressions for the second derivatives into the differentiated thermal isolation condition and coupling with the differentiated mechanical equilibrium condition gives the equations

$$\left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} \left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} + \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} = p_0(v) ,$$

and

$$p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) \left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} + \left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} =$$

$$(v - v_{p0}) [p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) - \frac{1}{2} p_0(v)] + (e - e_{p0}) \equiv e_0(v, e)$$

Solutions for the first derivatives of the product variables are, then,

$$\left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} = \frac{e_0(v, e) \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} - p_0(v)}{i_p(v_{p0}, e_{p0})},$$

and

$$\left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} = \frac{p_0(v) p_{Sr}(v; v_{rk}, e_{rk} + \Delta h_D) - e_0(v, e) \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p}}{i_p(v_{p0}, e_{p0})}.$$

The leading terms of the Taylor's series expansions for the reactant and product variables are

$$v_r = v + (v - v_{p0})\lambda + \left[(v - v_{p0}) - \left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} \right] \lambda^2 + \dots,$$

$$e_r = e + (e - e_{p0})\lambda + \left[(e - e_{p0}) - \left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} \right] \lambda^2 + \dots,$$

$$v_p = v_{p0} + \left[\left(\frac{\partial v_p}{\partial \lambda} \right)_{\lambda=0} \right] \lambda + \dots,$$

and

$$e_p = e_{p0} + \left[\left(\frac{\partial e_p}{\partial \lambda} \right)_{\lambda=0} \right] \lambda + \dots.$$

6. Method of Characteristics

FRONTIER uses characteristic compatibility conditions to couple the Riemann solutions for front propagation to the interior region solution. These must be modified to account for the effect of reaction (Grove 1998). Using a local coordinate system (\tilde{x}) directed normal to the front, the conditions applicable along streamlines are

$$\frac{\partial h}{\partial t} + \tilde{u} \frac{\partial h}{\partial \tilde{x}} = v \left(\frac{\partial p}{\partial t} + \tilde{u} \frac{\partial p}{\partial \tilde{x}} \right),$$

and

$$\frac{\partial \lambda}{\partial t} + \tilde{u} \frac{\partial \lambda}{\partial \tilde{x}} = \dot{\lambda}(\lambda, p, \dots).$$

Here, h is the enthalpy defined as

$$h = e + pv.$$

Further, the conditions

$$\frac{\partial p}{\partial t} + (\tilde{u} \pm c) \frac{\partial p}{\partial \tilde{x}} + \rho c \left(\frac{\partial \tilde{u}}{\partial t} + (\tilde{u} \pm c) \frac{\partial \tilde{u}}{\partial \tilde{x}} \right) = \left[(\rho c^2 - \Gamma p)(v_p - v_r) - \Gamma(e_p - e_r) \right] \rho \dot{\lambda}(\lambda, p, \dots)$$

are applicable along paths for which

$$\frac{d\tilde{x}}{dt} = \tilde{u} \pm c.$$

These equations contain a source term due to the presence of chemical reaction. In the absence of reaction, the compatibility equations of gas dynamics are recovered.

7. Summary and Conclusions

While there is still considerable controversy surrounding the validity of the assumptions of mechanical equilibrium and thermal isolation, they appear to represent the conditions prevalent during shock initiation of solid explosives with sufficient accuracy for use with a calibrated initiation model. Based on these assumptions, we have developed a discrete mixture equation of state for use with the gas dynamics conservation equations that takes advantage of the unique features offered by the front-tracking method. We have derived all of the additional thermodynamic expressions required to implement the mixture model in the front-tracking context. In addition to incomplete equations of state for pressure and temperature, these expressions include the sound speed and Grüneisen functions, the temperature and specific heat, along with adiabats and Hugoniot. We have recently completed implementation of this approach in *FRONTIER*.

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Appendix A:

Equations of State

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A-1. Equations of State and Constraints

A complete equation of state has the form

$$e = e(v, s),$$

such that

$$p(v, s) \equiv - \left(\frac{\partial e}{\partial v} \right)_s$$

and

$$T(v, s) \equiv \left(\frac{\partial e}{\partial s} \right)_v,$$

where e is specific internal energy, v is specific volume, s is specific entropy, p is pressure, and T is temperature. The expressions for pressure and temperature each represent incomplete equations of state. By solving the complete equation of state for entropy and substituting into the incomplete equations of state, the latter are represented as functions of specific volume and internal energy. An incomplete equation of state giving pressure in the form,

$$p = p(v, e),$$

as required by the gas dynamics conservation equations can be represented by a surface in p - v - e space. The partial derivative of the equation-of-state pressure with respect to internal energy is, generally, a positive function of both specific volume and internal energy denoted by

$$\left(\frac{\partial p}{\partial e} \right)_v = p_\Gamma(v, e) > 0.$$

Any constraint (e.g., constant temperature, constant entropy, etc.) on the processes that the material described by that equation of state may undergo can similarly be represented by such a surface. The intersection of the two surfaces defines a path along which the constrained states must lie. Along this path, each of the variables (p , v , or e) may be represented as a function of either of the other two variables. For example,

$$e = e_R(v),$$

and

$$p = p_R(v),$$

where the subscript is chosen to identify the particular constraint.

It is possible to develop an equation of state if equations describing a constrained path and a transverse derivative on that path are known. For example, if the derivative of pressure with respect to internal energy,

$$\left(\frac{\partial p}{\partial e} \right)_R = \rho_T[v, e_R(v)],$$

is known on a path as a function of specific volume, an equation of state valid near the path is given by

$$p(v, e) = p_R(v) + \rho_T[v, e_R(v)][e - e_R(v)].$$

The validity of this expression is extended to points arbitrarily far from the path if the derivative is everywhere independent of internal energy. That is, the derivative must be a function of the specific volume only. In this case, the equation of state may be written

$$p(v, e) = p_R(v) + \rho_\Gamma(v) [e - e_R(v)].$$

Using the Grüneisen function, defined as

$$\Gamma(v) = v \left(\frac{\partial p}{\partial e} \right)_v = \rho_\Gamma(v) v,$$

the Mie-Grüneisen equation of state is written

$$p(v, e) = p_R(v) + \frac{\Gamma(v)}{v} [e - e_R(v)].$$

With appropriate reference and Grüneisen functions, it represents a wide variety of commonly used equations of state that are linear in the specific internal energy. (A notable exception, offered by Davis [1993], is an equation of state for detonation products that is quadratic in the internal energy.)

It is often convenient to write these linear equations of state in the form

$$p(v, e) = p_\Gamma(v) + \rho_\Gamma(v) e,$$

where

$$\rho_\Gamma(v) = \frac{\Gamma(v)}{v}$$

is a representation of the Grüneisen function and

$$p_\Gamma(v) = p_R(v) - \rho_\Gamma(v) e_R(v)$$

combines the reference and Grüneisen functions.

Solving for the specific internal energy gives

$$e(p, v) = e_R(v) + \frac{v[p - p_R(v)]}{\Gamma(v)} = \frac{p - p_r(v)}{\rho_r(v)} = p v_r(v) - e_r(v),$$

where

$$v_r(v) = \frac{1}{\rho_r(v)},$$

and

$$e_r(v) = p_r(v) v_r(v).$$

A-2. Isentropes

When the constraint is the condition of constant entropy, the path is known as an isentrope. If (v_k, e_k) is a known state on an isentrope, then the equation

$$e = e[v, s(v_k, e_k)] = e_S(v; v_k, e_k)$$

describes the variation in specific internal energy with specific volume along the isentrope. Because of the fundamental thermodynamic identity,

$$de = Tds - pdv,$$

the pressure and internal energy have a special relation along an isentrope ($ds=0$):

$$\frac{de_S}{dv} = -p_S(v; v_k, e_k) = -p[v, e_S(v; v_k, e_k)] .$$

This constitutes a first-order ordinary differential equation for $e_S(v; v_k, e_k)$. In this most general form, it defies solution.

As we have noted, many equations of state of practical interest are linear in the internal energy. In this case, the differential equation can be written

$$\frac{de_S}{dv} + \rho_T(v) e_S(v; v_k, e_k) = -\rho_T(v) ,$$

and a family of solutions can be found using an integrating factor (depending only on the form of the Grüneisen function) given by

$$f_S(v) = \exp \left(\int_{v_0}^v \rho_T(v) dv \right) ,$$

where v_0 is an arbitrary reference volume. Defining

$$g_S(v) - g_S(v_k) = - \int_{v_k}^v f_S(v) \rho_T(v) dv ,$$

the solutions, (which are independent of v_0) are

$$e_S(v; v_k, e_k) = \frac{g_S(v) - g_S(v_k) + f_S(v_k) e_k}{f_S(v)} \equiv \frac{g_S(v) + a_{sk}}{f_S(v)} .$$

Thus, each isentrope may be described using the single constant, a_{sk} :

$$a_S(v, e) \equiv f_S(v) e - g_S(v) = f_S(v_k) e_k - g_S(v_k) = a_S(v_k, e_k) \equiv a_{sk} .$$

Defining

$$h_S(v) \equiv \frac{g_S(v)}{f_S(v)} ,$$

we may write

$$e_S(v; v_k, e_k) = h_S(v) + \frac{f_S(v_k)}{f_S(v)} [e_k - h_S(v_k)] = h_S(v) + \frac{a_{sk}}{f_S(v)}$$

and

$$a_S(v, e) \equiv f_S(v) [e - h_S(v)] = f_S(v_k) [e_k - h_S(v_k)] = a_S(v_k, e_k) \equiv a_{sk} .$$

If the form of the isentrope is known such that $f_S(v)$ along with $g_S(v)$ or $h_S(v)$ can be identified, an equation of state can be determined by differentiating. Thus,

$$\rho_T(v) = \frac{1}{f_S(v)} \frac{df_S}{dv}$$

and

$$\rho_T(v) = \frac{-1}{f_S(v)} \frac{dg_S}{dv} = - \frac{dh_S}{dv} - \rho_T(v) h_S(v) .$$

The equation of state thus obtained is independent of the state (v_k, e_k) , (i.e., valid on any isentrope). Under these conditions, the reference curve provides all the information necessary to construct the equation of state, including the Grüneisen function.

We can determine the pressure on the isentrope by substituting into the equation of state or by differentiating $e_S(v; v_k, e_k)$:

$$p_S(v; v_k, e_k) = \frac{1}{f_S(v)} \left(\frac{g_S(v) + a_{sk}}{f_S(v)} \frac{df_S}{dv} - \frac{dg_S}{dv} \right),$$

or, alternatively,

$$p_S(v; v_k, e_k) = \frac{a_{sk}}{v_S(v)} - \frac{dh_S}{dv},$$

where

$$v_S(v) = \frac{f_S(v)}{\rho_r(v)}.$$

We shall also have use for the differential equation satisfied by $p_S(v; v_k, e_k)$. It can be obtained by differentiating the isentrope pressure and substituting for the isentrope energy from the equation of state, giving

$$\frac{dp_S}{dv} + \rho_r(v) \frac{d}{dv} [v + v_r(v)] p_S(v; v_k, e_k) = \rho_r(v) \frac{de_r}{dv}.$$

The integrating factor associated with this equation is $v_S(v)$, which, again, depends only on the form of the Grüneisen function.

We can also relate the isentrope to the reference functions. Substituting for $p_r(v)$ gives

$$g_S(v) - g_S(v_k) = \int_{v_k}^v f_S(v) \rho_r(v) e_R(v) dv - \int_{v_k}^v f_S(v) p_R(v) dv.$$

Noting that

$$\frac{df_S}{dv} = f_S(v) \rho_r(v),$$

the first term of this equation can be integrated by parts. Thus,

$$g_S(v) - g_S(v_k) = g_R(v) - g_R(v_k) + f_S(v) e_R(v) - f_S(v_k) e_R(v_k),$$

where

$$g_R(v) - g_R(v_k) = - \int_{v_k}^v f_S(v) \left(p_R(v) + \frac{de_R}{dv} \right) dv.$$

This gives

$$e_S(v; v_k, e_k) = e_R(v) + \frac{g_R(v) - g_R(v_k) + f_S(v_k)[e_k - e_R(v_k)]}{f_S(v)} \equiv e_R(v) + \frac{g_R(v) + a_{rk}}{f_S(v)}$$

for the isentrope energy and

$$p_S(v; v_k, e_k) = p_R(v) + \frac{g_R(v) - g_R(v_k) + f_S(v_k)[e_k - e_R(v_k)]}{v_S(v)} \equiv p_R(v) + \frac{g_R(v) + a_{rk}}{v_S(v)}$$

for the isentrope pressure.

The derivative of the isentrope pressure is the square of the acoustic impedance:

$$i_S^2(v; v_k, e_k) = - \frac{dp_S}{dv} = p_\Gamma(v) \left[\left(1 + \frac{dv_\Gamma}{dv} \right) p_S(v; v_k, e_k) - \frac{de_\Gamma}{dv} \right].$$

It must remain positive.

A-3. Sound-Speed Functions

By differentiating the equation of state in the form

$$p(v, s) = p_r(v) + \rho_r(v) e(v, s),$$

the square of the acoustic impedance can be expressed as a function of state:

$$i^2(v, s) = - \left(\frac{\partial p}{\partial v} \right)_s = \left(\frac{p_r(v)}{v_r(v)} - \frac{dp_r}{dv} \right) + \left(\frac{\rho_r(v)}{v_r(v)} - \frac{d\rho_r}{dv} \right) e(v, s).$$

The square of the sound speed and the adiabatic exponent are given by

$$c^2(v, s) = v^2 i^2(v, s),$$

and

$$\gamma(v, s) = \frac{v i^2(v, s)}{p(v, s)}.$$

These may also be expressed as functions of v and e :

$$i^2(v, e) = \left(\frac{p_r(v)}{v_r(v)} - \frac{dp_r}{dv} \right) + \left(\frac{\rho_r(v)}{v_r(v)} - \frac{d\rho_r}{dv} \right) e,$$

$$c^2(v, e) = v^2 i^2(v, e),$$

and

$$\gamma(v, e) = \frac{v i^2(v, e)}{p(v, e)} .$$

These functions must remain positive in order to prevent imaginary sound speeds.

A-4. Completing the Equation of State

A complete equation of state can be determined if, in addition to the incomplete equation of state for pressure, an incomplete equation of state for temperature,

$$T = T(v, e) ,$$

is developed using suitable assumptions. Following Grove (1997), we solve the pressure equation of state for energy, giving

$$e = \frac{p - p_r(v)}{\rho_r(v)} = p v_r(v) - e_r(v) ,$$

so that the specific internal energy differential is

$$de = v_r(v) dp + p \frac{dv_r}{dv} dv - \frac{de_r}{dv} dv .$$

Substituting into the differential of the complete equation of state,

$$de = T ds - p dv ,$$

and rearranging gives

$$T ds = v_r(v) dp + p \frac{d}{dv} [v + v_r(v)] dv - \frac{de_r}{dv} dv .$$

Introducing a fictitious pressure, $p_*(v)$, we may write

$$T ds = \left(v_f(v) \frac{dp_\infty}{dv} + \frac{d}{dv} [v + v_f(v)] p_\infty(v) - \frac{de_f}{dv} dv \right) dv \\ + [p - p_\infty(v)] \frac{d}{dv} [v + v_f(v)] dv + v_f(v) d[p - p_\infty(v)]$$

The leading term on the right-hand side of this expression has been shown to vanish for

$$p_\infty(v) = p_s(v; v_\infty, e_\infty),$$

where (v_∞, e_∞) , is a suitable reference state. Denoting $p - p_\infty(v)$, referred to as the stiff pressure, by p^* , we may write

$$T(p^*, v) ds = p^* \frac{d}{dv} [v + v_f(v)] dv + v_f(v) dp^*.$$

Assuming temperature in the form,

$$T(p^*, v) = T_v(p^*) T_{p^*}(v),$$

gives

$$ds = \frac{p^* \frac{d}{dv} [v + v_f(v)] dv}{T_v(p^*) T_{p^*}(v)} + \frac{v_f(v) dp^*}{T_v(p^*) T_{p^*}(v)}.$$

Thus,

$$\left(\frac{\partial s}{\partial v} \right)_{p^*} = \frac{p^* \frac{d}{dv} [v + v_f(v)]}{T_v(p^*) T_{p^*}(v)}$$

and

$$\left(\frac{\partial s}{\partial p^*} \right)_v = \frac{v_\Gamma(v)}{T_v(p^*) T_{p^*}(v)} .$$

Cross differentiating gives

$$\frac{\partial^2 s}{\partial p^* \partial v} = \frac{1}{T_{p^*}(v)} \frac{d}{dv} [v + v_\Gamma(v)] \frac{d}{dp^*} \left(\frac{p^*}{T_v(p^*)} \right) = \frac{1}{T_v(p^*)} \frac{d}{dv} \left(\frac{v_\Gamma(v)}{T_{p^*}(v)} \right)$$

or

$$T_v(p^*) \frac{d}{dp^*} \left(\frac{p^*}{T_v(p^*)} \right) = \frac{T_{p^*}(v) \frac{d}{dv} \left(\frac{v_\Gamma(v)}{T_{p^*}(v)} \right)}{\frac{d}{dv} [v + v_\Gamma(v)]} = 1 - w ,$$

where w is a constant, and two differential equations result. The equation for $T_v(p^*)$ is

$$\frac{dT_v}{dp^*} - \frac{w}{p^*} T_v(p^*) = 0 ,$$

and a solution is

$$T_v(p^*) = \left(\frac{p^*}{RT_0} \right)^w ,$$

where RT_0 is a constant. The equation for $T_{p^*}(v)$ is

$$\frac{dT_{p^*}}{dv} + \left((1-w) \rho_\Gamma(v) + \frac{w}{\rho_\Gamma(v)} \frac{d\rho_\Gamma}{dv} \right) T_{p^*}(v) = 0 ,$$

and a solution is

$$T_{p^*}(v) = \frac{\Gamma_o T_o [f_S(v)]^{w-1}}{[\rho_r(v)]^w} = \Gamma_o T_o \frac{[v_S(v)]^w}{f_S(v)},$$

where $\Gamma_o T_o$ is a constant. Thus,

$$T(p, v) = \frac{\Gamma_o T_o}{f_S(v)} \left(\frac{v_S(v) [p - p_S(v; v_\infty, e_\infty)]}{RT_o} \right)^w,$$

and, substituting for pressure,

$$\begin{aligned} T(v, e) &= \frac{\Gamma_o T_o}{f_S(v)} \left(\frac{f_S(v) [\rho_r(v) + \rho_r(v) e - p_S(v; v_\infty, e_\infty)]}{RT_o \rho_r(v)} \right)^w \\ &= \frac{\Gamma_o T_o}{f_S(v)} \left(\frac{[e - e_S(v; v_\infty, e_\infty)] f_S(v)}{RT_o} \right)^w. \end{aligned}$$

Here, the reference state (v_∞, e_∞) , along with the exponent w , may be chosen for consistency with known or assumed forms of the temperature. Solving for internal energy gives

$$e(T, v) = \frac{RT_o}{f_S(v)} \left(\frac{f_S(v)}{\Gamma_o} \frac{T}{T_o} \right)^{1/w} + e_S(v; v_\infty, e_\infty),$$

and the specific heat at constant volume is

$$c_v(T, v) = \left(\frac{\partial e}{\partial T} \right)_v = \frac{R}{w \Gamma_o} \left(\frac{f_S(v)}{\Gamma_o} \frac{T}{T_o} \right)^{(1-w)/w}.$$

This is inconsistent with results from quantum statistical mechanics, which show that c_v has no volume dependence and is bounded for large temperatures (Vincenti and Kruger 1967; Callen 1960). However, for polyatomic gases at low and very high temperatures and for solids at very high temperatures, c_v is nearly constant, corresponding to $w = 1$. In this case,

$$c_v = \frac{R}{\Gamma_0} = c_{v0},$$

and the temperature is given by

$$T(p, v) = \frac{p - p_S(v; v_\infty, e_\infty)}{c_{v0} \rho_\Gamma(v)},$$

or

$$\begin{aligned} T(v, e) &= \frac{e - e_S(v; v_\infty, e_\infty)}{c_{v0}} \\ &= \frac{f_S(v)[e - h_S(v)] - f_S(v_\infty)[e_\infty - h_S(v_\infty)]}{c_{v0} f_S(v)} = \frac{a_S(v, e) - a_{S\infty}}{c_{v0} f_S(v)}. \end{aligned}$$

Note that the temperature vanishes everywhere along the isentrope through (v_∞, e_∞) . Properly, then, this isentrope should be the "cold compression curve" given by

$$p_C(v) = p_S(v; v_\infty, e_\infty)$$

or

$$e_C(v) = e_S(v; v_\infty, e_\infty),$$

where $e_C(v)$ is the specific interatomic potential energy. As a practical alternative, $a_{S\infty}$ may be determined with reference to a known temperature. If T_j is the known temperature at the state (v_j, e_j) , then the expression

$$a_{S\infty} = a_{sj} - f_S(v_j) c_{v0} T_j$$

constrains the state (v_∞, e_∞) . In this case, the proper behavior at cold temperatures may not be realized.

The temperature on an isentrope is given by

$$T_S(v; v_k, e_k) = \frac{p_S(v; v_k, e_k) - p_S(v; v_\infty, e_\infty)}{c_{vo} \rho_\Gamma(v)} = \frac{e_S(v; v_k, e_k) - e_S(v; v_\infty, e_\infty)}{c_{vo}}.$$

Specific entropy in the form,

$$s(p^*, v) = c_{vo} \log \left(\frac{p^* v_S(v)}{RT_o} \right),$$

satisfies

$$\left(\frac{\partial s}{\partial v} \right)_{p^*} = \frac{p^* \frac{d}{dv} [v + v_\Gamma(v)]}{T(p^*, v)} = \frac{c_{vo}}{v_S(v)} \frac{dv_S}{dv}$$

and

$$\left(\frac{\partial s}{\partial p^*} \right)_v = \frac{v_\Gamma(v)}{T(p^*, v)} = \frac{c_{vo}}{p^*}$$

but violates the Nernst postulate. The complete equation of state is

$$e(v, s) = \frac{RT_o}{f_S(v)} \exp \left(\frac{s}{c_{vo}} \right) + e_C(v).$$

A-5. Hugoniot

We have shown that an isentrope can be used to determine an equation of state. A shock Hugoniot is another path in the p - v plane that is used in equations of state. Rather than describing a process, it represents the locus of all possible states on the downstream side of a shock wave for a specified upstream state.

If U denotes the shock propagation velocity and u the component of the particle velocity normal to the shock wave, the equations expressing conservation of mass, momentum, and energy across the shock wave may be written

$$\Delta^u v (U - u_u) = v_u \Delta^u u,$$

$$(U - u_u) \Delta^u u = \Delta^u p v_u,$$

and

$$\Delta^u e + \Delta^u (p v) = (U - u_u) \Delta^u u - \frac{1}{2} (\Delta^u u)^2.$$

Here, unsubscripted variables refer to the downstream state, and the subscript u denotes known conditions on the upstream side of the shock wave. The operator Δ^u represents changes across the shock:

$$\Delta^u q = q - q_u.$$

For convenience, we also define

$${}^u\Delta v = v_u - v.$$

Eliminating $U - u_u$ between the mass and momentum conservation equations gives

$$(\Delta^u u)^2 = \Delta^u p {}^u\Delta v.$$

Substituting the expressions for $(U - u_u) \Delta^u u$ and $(\Delta^u u)^2$ into the energy equation gives the Hugoniot relation:

$$\Delta^u e = (p_u + \frac{1}{2} \Delta^u p) \Delta^u v.$$

This represents a surface in p - v - e space. The intersection of this surface with the equation-of-state surface is obtained by inverting the equation of state to give specific internal energy as a function of pressure and specific volume and substituting into the foregoing equation. Noting that the upstream material may be described by a different equation of state (e.g., due to chemical reaction), this gives

$$e(p, v) - e_u(p_u, v_u) = (p_u + \frac{1}{2} \Delta^u p) \Delta^u v,$$

which represents a Hugoniot in the p - v plane. In principle, this can be written

$$p = p_H(v; p_u, v_u),$$

or, alternatively,

$$\Delta^u p = \Delta^u p_H(v; p_u, v_u).$$

The Hugoniot energy is related to the Hugoniot pressure by the Hugoniot relation:

$$e_H(v; p_u, v_u) = e_u(p_u, v_u) + \frac{1}{2} [p_u + p_H(v; p_u, v_u)] \Delta^u v,$$

or

$$\Delta^u e_H(v; p_u, v_u) = [p_u + \frac{1}{2} \Delta^u p_H(v; p_u, v_u)] \Delta^u v.$$

This may be differentiated to give

$$\frac{de_H}{dv} = \frac{1}{2} \left({}^u\Delta v \frac{dp_H}{dv} - p_u - p_H(v; p_u, v_u) \right) = \frac{1}{2} \left({}^u\Delta v \frac{dp_H}{dv} - \Delta^u p_H(v; p_u, v_u) \right) - p_u .$$

For an equation of state that is linear in internal energy, we may write

$$p_H(v; p_u, v_u) = \frac{p_\Gamma(v) + [1 - f_H(v; v_u)] p_u + \rho_\Gamma(v) e_u(p_u, v_u)}{f_H(v; v_u)} ,$$

or

$$\Delta^u p_H(v; p_u, v_u) = \frac{p_\Gamma(v) - p_u + \rho_\Gamma(v) [e_u(p_u, v_u) + p_u {}^u\Delta v]}{f_H(v; v_u)} ,$$

for the Hugoniot pressure. Here the Hugoniot factor is defined as

$$f_H(v; v_u) = 1 - \frac{1}{2} \rho_\Gamma(v) {}^u\Delta v .$$

Hugoniots are valid in compression ($v \leq v_u$) only and may be thought of as emanating from the upstream state. If the Hugoniot factor vanishes, there may also be a lower limit on the specific volume that may be obtained by shock compression. Thus,

$$\rho_\Gamma(v) = \frac{\Gamma(v)}{v} < \frac{2}{{}^u\Delta v} .$$

Segletes (1991) has identified this inequality as a stability requirement for the Hugoniot-referenced Mie-Grüneisen equation of state. The minimum specific volume is obtained by solving the equation

$$\rho_\Gamma(v_{min}) = \frac{2}{v_u - v_{min}} .$$

The Hugoniot pressure and energy become unbounded as the specific volume approaches this minimum. This singularity is due only to the form of the Grüneisen function.

The Hugoniot and isentrope functions for an equation of state that is linear in internal energy are related by the expression

$$p_S(v; v_k, e_k) = p_H(v; p_u, v_u) + \rho_r(v) [e_S(v; v_k, e_k) - e_H(v; p_u, v_u)].$$

Differentiating gives

$$\begin{aligned} \frac{dp_S}{dv} &= f_H(v; v_u) \frac{dp_H}{dv} + \rho_r(v) \left[\frac{1}{2} \Delta^u p_H(v; p_u, v_u) - p_S(v; v_k, e_k) + p_H(v; p_u, v_u) \right] \\ &\quad + \frac{d\rho_r}{dv} [e_S(v; v_k, e_k) - e_H(v; p_u, v_u)]. \end{aligned}$$

Thus, the derivative of the isentrope at the Hugoniot is

$$\left. \frac{dp_S}{dv} \right|_H = f_H(v; v_u) \frac{dp_H}{dv} + \frac{1}{2} \rho_r(v) \Delta^u p_H(v; p_u, v_u).$$

Evaluated at the upstream state, this becomes

$$\left. \frac{dp_S}{dv} \right|_u = \left. \frac{dp_H}{dv} \right|_u,$$

showing that the Hugoniot and isentrope are tangent as they pass through that state.

A-6. The Grüneisen Function

The Grüneisen function is commonly represented in the linear form (Steinberg, Cochran, and Guinan 1980)

$$\Gamma(v) = \Gamma_o + \rho_{\Gamma_o} v ,$$

so that

$$\rho_{\Gamma}(v) = \frac{\Gamma(v)}{v} = \rho_{\Gamma_o} + \frac{\Gamma_o}{v} .$$

The integrating factor for the isentrope energy becomes

$$f_S(v) = \exp \left(\int_{v_o}^v \rho_{\Gamma}(v) dv \right) = (v/v_o)^{\Gamma_o} \exp[\rho_{\Gamma_o}(v-v_o)] .$$

The derivative of $\rho_{\Gamma}(v)$ is

$$\frac{d\rho_{\Gamma}}{dv} = - \frac{\Gamma_o}{v^2} ,$$

and the square of the acoustic impedance may be written

$$i^2(v, e) = \left(\rho_{\Gamma_o} + \frac{\Gamma_o}{v} \right) \rho_{\Gamma}(v) - \frac{d\rho_{\Gamma}}{dv} + \left[\frac{\rho_{\Gamma_o}}{v_{\Gamma_o}} + \frac{2\Gamma_o \rho_{\Gamma_o}}{v} + \frac{\Gamma_o(\Gamma_o+1)}{v^2} \right] e .$$

The complete equation of state is

$$e(v, s) = RT_o \left(\frac{v_o}{v} \right)^{\Gamma_o} \exp \left(\frac{s}{c_{v_o}} - \frac{v}{v_{\Gamma_o}} \right) + e_S(v; v_{\infty}, e_{\infty}) ,$$

where

$$v_{\Gamma_o} \equiv \frac{1}{\rho_{\Gamma_o}} .$$

With $\rho_{\Gamma_o}=0$, the Grüneisen function is constant, and, with $\Gamma_o=0$, it is proportional to the specific volume. We shall find it useful to specialize some of the expressions derived in the foregoing sections to these cases.

A-6.1 Constant Grüneisen Function. The simplest form of the Grüneisen function is the constant- Γ form ($\rho_{\Gamma_o}=0$):

$$\rho_{\Gamma}(v) = \frac{\Gamma(v)}{v} = \frac{\Gamma_o}{v} .$$

Differentiating gives

$$\frac{d\rho_{\Gamma}}{dv} = -\frac{\Gamma_o}{v^2} .$$

The isentrope energy and pressure integrating factors become

$$f_S(v) = (v/v_o)^{\Gamma_o} ,$$

and

$$v_S(v) = \frac{f_S(v)}{\rho_{\Gamma}(v)} = \frac{v(v/v_o)^{\Gamma_o}}{\Gamma_o} .$$

The square of the acoustic impedance is

$$i^2(v, e) = \left(\frac{\Gamma_o \rho_{\Gamma}(v)}{v} - \frac{d\rho_{\Gamma}}{dv} \right) + \frac{\Gamma_o(\Gamma_o+1)}{v^2} e .$$

The Hugoniot factor and minimum specific volume are

$$f_H(v; v_u) = 1 - \Gamma_o \frac{u \Delta v}{2v} ,$$

and

$$v_{min} = \frac{\Gamma_o}{\Gamma_o + 2} v_u .$$

The complete equation of state is

$$e(v, s) = RT_o \left(\frac{v_o}{v} \right)^{\Gamma_o} \exp \left(\frac{s}{c_{vo}} \right) + e_S(v; v_\infty, e_\infty) .$$

A-6.2 Proportional Grüneisen Function. Another simple form of the Grüneisen function is the proportional form ($\Gamma_o = 0$):

$$\rho_\Gamma(v) = \frac{\Gamma(v)}{v} = \rho_{\Gamma_o} \equiv \frac{1}{v_{\Gamma_o}} ,$$

where ρ_{Γ_o} is a constant and the derivative of $\rho_\Gamma(v)$ vanishes. The isentrope energy and pressure integrating factors become

$$f_S(v) = \exp[\rho_{\Gamma_o}(v - v_o)] ,$$

and

$$v_S(v) = \frac{f_S(v)}{\rho_\Gamma(v)} = \frac{\exp[\rho_{\Gamma_o}(v - v_o)]}{\rho_{\Gamma_o}} .$$

The square of the acoustic impedance is

$$i^2(v, e) = \left(\rho_{\Gamma_o} \rho_{\Gamma}(v) - \frac{d\rho_{\Gamma}}{dv} \right) + \rho_{\Gamma_o}^2 e.$$

The Hugoniot factor and minimum specific volume are

$$f_H(v; v_u) = \left(1 - \frac{1}{2} \rho_{\Gamma_o}^u \Delta v \right),$$

and

$$v_{min} = v_u - 2 v_{\Gamma_o}.$$

The complete equation of state is

$$e(v, s) = RT_o \exp \left(\frac{s}{c_{vo}} - \frac{v}{v_{\Gamma_o}} \right) + e_S(v; v_{\infty}, e_{\infty}).$$

A-7. Polytropic Gas Equation of State

A-7.1 Incomplete Equation of State for Pressure. With a constant Grüneisen coefficient, $\Gamma_o = \gamma_o - 1$, and reference to zero pressure and internal energy, the polytropic gas equation of state results:

$$p(v, e) = \frac{\gamma_o - 1}{v} e.$$

The function $\rho_{\Gamma}(v)$ may be identified as

$$\rho_r(v) = \frac{\gamma_0 - 1}{v},$$

and $p_r(v)$ vanishes.

A-7.2 Isentrope. Thus, the integrating factor for the isentrope energy is

$$f_S(v) = \exp \left[(\gamma_0 - 1) \int_{v_0} \frac{dv}{v} \right] = \exp [(\gamma_0 - 1) \log(v/v_0)] = (v/v_0)^{\gamma_0 - 1}.$$

The function $g_S(v)$ vanishes. The internal energy and pressure on the isentrope are, then, given by

$$e_S(v; v_k, e_k) = \frac{f_S(v_k)}{f_S(v)} e_k = (v_k/v)^{\gamma_0 - 1} e_k,$$

and

$$p_S(v; v_k, e_k) = \frac{f_S(v_k)}{f_S(v)} e_k \rho_r(v) = \frac{\gamma_0 - 1}{v_k} e_k (v_k/v)^{\gamma_0} = p_k (v_k/v)^{\gamma_0}.$$

Thus, on an isentrope,

$$v^{\gamma_0 - 1} e = v_k^{\gamma_0 - 1} e_k,$$

and

$$p v^{\gamma_0} = p_k v_k^{\gamma_0}.$$

A-7.3 Sound-Speed Functions. The square of the acoustic impedance is

$$j^2 = \left(\frac{\rho_r(v)}{v_r(v)} - \frac{d\rho_r}{dv} \right) e = \frac{\gamma_o(\gamma_o - 1)}{v^2} e = \frac{\gamma_o}{v} p ,$$

the square of the sound speed is

$$c^2 = v^2 j^2 = \gamma_o(\gamma_o - 1) e = \gamma_o p v ,$$

and the adiabatic exponent is

$$\gamma = \frac{c^2}{p v} = \gamma_o .$$

These are positive for positive specific internal energy.

A-7.4 Complete Equation of State. The temperature of a polytropic gas is known to vanish for vanishing specific internal energy. This is consistent with a vanishing specific interatomic potential energy:

$$e_C(v) = e_S(v; v_\infty, e_\infty) = 0 ,$$

which implies that

$$v_\infty^{\gamma_o - 1} e_\infty = 0 ,$$

and

$$p_C(v) = p_S(v; v_\infty, e_\infty) = 0 .$$

Thus, the stiff pressure is simply equal to the pressure, and the temperature is given by

$$T = \frac{e}{c_{vo}} = \frac{p v}{R} = \frac{\gamma_o - 1}{R} e .$$

The integrating factor for the isentrope pressure is

$$v_S(v) = \frac{f_S(v)}{\rho_T(v)} = \frac{v(v/v_0)^{\gamma_0-1}}{\gamma_0-1}.$$

The entropy may then be written

$$s = c_{vo} \log \left(\frac{p v (v/v_0)^{\gamma_0-1}}{(\gamma_0-1) R T_0} \right) = c_{vo} \log \left(\frac{p v^{\gamma_0}}{\rho_0 v_0^{\gamma_0}} \right) = c_{vo} \log \left(\frac{v^{\gamma_0-1} e}{v_0^{\gamma_0-1} e_0} \right),$$

where

$$e_0 = R T_0$$

and

$$\rho_0 = (\gamma_0-1) \frac{e_0}{v_0},$$

and the complete equation of state is

$$e = R T_0 \left(\frac{v_0}{v} \right)^{\gamma_0-1} \exp \left(\frac{s}{c_{vo}} \right).$$

A-7.5 Hugoniot. The Hugoniot factor is

$$f_H(v; v_u) = 1 - \frac{1}{2} \rho_T(v) u \Delta v = 1 - \frac{\gamma_0-1}{2v} (v_u - v),$$

and the Hugoniot pressure is given by

$$p_H(v; p_u, v_u) = \frac{(\gamma_o + 1) v_u - (\gamma_o - 1) v}{(\gamma_o + 1) v - (\gamma_o - 1) v_u} p_u.$$

The minimum specific volume is

$$v_{min} = \frac{\gamma_o - 1}{\gamma_o + 1} v_u.$$

A-8. Stiffened Polytropic Gas Equation of State

A-8.1 Incomplete Equation of State for Pressure. The polytropic gas equation of state is “stiffened” by the use of a constant pressure reference:

$$p_R(v) = \gamma_o p_\infty,$$

so that

$$p(v, e) = \gamma_o p_\infty + \frac{\gamma_o - 1}{v} e.$$

The function $p_r(v)$ remains unchanged while

$$p_r(v) = \gamma_o p_\infty.$$

A-8.2 Isentrope. The integrating factor for the isentrope energy remains unchanged and

$$g_S(v) = -p_\infty v_o (v/v_o)^{\gamma_o}.$$

The internal energy and pressure along the isentrope are, then, given by

$$e_S(v; v_k, e_k) = [(p_\infty + e_k/v_k)(v_k/v)^{\gamma_0} - p_\infty] v,$$

and

$$p_S(v; v_k, e_k) = p_\infty + (\gamma_0 - 1)(p_\infty + e_k/v_k)(v_k/v)^{\gamma_0}.$$

Thus, on an isentrope,

$$(p_\infty + e/v) v^{\gamma_0} = (p_\infty + e_k/v_k) v_k^{\gamma_0},$$

and

$$(p - p_\infty) v^{\gamma_0} = (p_k - p_\infty) v_k^{\gamma_0}.$$

A-8.3 Sound-Speed Functions. The square of the acoustic impedance is

$$j^2 = \left(\frac{p_\Gamma(v)}{v_\Gamma(v)} - \frac{dp_\Gamma}{dv} \right) + \left(\frac{p_\Gamma(v)}{v_\Gamma(v)} - \frac{dp_\Gamma}{dv} \right) e = \frac{\gamma_0(\gamma_0 - 1)}{v} \left(p_\infty + \frac{e}{v} \right) = \frac{\gamma_0 - 1}{v} \left(p + \frac{e}{v} \right),$$

the square of the sound speed is

$$c^2 = v^2 j^2 = \gamma_0(\gamma_0 - 1)(p_\infty v + e),$$

and the adiabatic exponent is

$$\gamma = \frac{c^2}{pv} = \frac{\gamma_0(\gamma_0 - 1)(p_\infty v + e)}{\gamma_0(p_\infty v + e) + e}.$$

A-8.4 Complete Equation of State. Choosing (v_∞, e_∞) so that

$$\frac{e_\infty}{v_\infty} = -p_\infty ,$$

associates p_∞ with the “cold pressure”:

$$p_C(v) = p_S(v; v_\infty, e_\infty) = p_\infty .$$

The resulting specific interatomic potential energy is

$$e_C(v) = e_S(v; v_\infty, e_\infty) = -p_\infty v .$$

Thus, the stiff pressure is

$$p^* = p - p_\infty ,$$

and the temperature may be written

$$T = \frac{p^* v}{R} = \frac{e + p_\infty v}{c_{v0}} .$$

The integrating factor, $v_S(v)$, for the isentrope pressure is unchanged and the specific entropy is given by

$$s(p, v) = c_{v0} \log \left(\frac{(p - p_\infty) v (v/v_0)^{\gamma_0 - 1}}{(\gamma_0 - 1) R T_0} \right) = c_{v0} \log \left(\frac{(p - p_\infty) v^{\gamma_0}}{(p_0 - p_\infty) v_0^{\gamma_0}} \right) ,$$

or

$$s(v, e) = c_{v0} \log \left(\frac{v^{\gamma_0 - 1} (e + p_\infty v)}{v_0^{\gamma_0 - 1} (e_0 + p_\infty v_0)} \right) ,$$

where

$$e_o = RT_o - p_\infty v_o ,$$

and

$$p_o = \gamma_o p_\infty + (\gamma_o - 1) \frac{e_o}{v_o} ,$$

and the complete equation of state is

$$e = RT_o \left(\frac{v_o}{v} \right)^{\gamma_o - 1} \exp \left(\frac{s}{c_{vo}} \right) - p_\infty v .$$

A-8.5 Hugoniot. The Hugoniot factor and the minimum specific volume remain unchanged from the polytropic gas case, and the Hugoniot pressure is given by

$$p_H(v; p_u, v_u) = \frac{[(\gamma_o + 1)v_u - (\gamma_o - 1)v] p_u - 2\gamma_o p_\infty (v_u - v)}{(\gamma_o + 1)v - (\gamma_o - 1)v_u} .$$

A-9. JWL Equation of State

A-9.1 Incomplete Equation of State for Pressure. In the case of the JWL equation of state, commonly applied to detonation products, we begin with a knowledge of the isentrope emanating from the Chapman-Jouget state, (v_j, e_j) . Lee and Hornig (1969) chose the form

$$e_S(v; v_j, e_j) = h_S(v) + \frac{e_j - h_S(v_j)}{(v/v_j)^\omega},$$

so that

$$p_S(v; v_j, e_j) = -\frac{dh_S}{dv} + \frac{\omega}{v} \frac{e_j - h_S(v_j)}{(v/v_j)^\omega},$$

where

$$h_S(v) = e_1 \exp(-\rho_1 v) + e_2 \exp(-\rho_2 v),$$

and

$$-\frac{dh_S}{dv} = \rho_1 \exp(-\rho_1 v) + \rho_2 \exp(-\rho_2 v).$$

Here,

$$e_m \equiv \frac{p_m}{\rho_m} \quad m=1,2,$$

and $\rho_1, \rho_2, \rho_1, \rho_2$, and ω are constants that are determined with reference to cylinder expansion test pressure-volume data. By comparison with our general solution for the isentrope energy, we see that this corresponds to a constant Grüneisen coefficient, $\Gamma_0 = \omega$, and

$$f_S(v) = (v/v_0)^\omega.$$

Thus,

$$\rho_\Gamma(v) = \frac{\Gamma(v)}{v} = \frac{1}{f_S(v)} \frac{df_S}{dv} = \frac{\omega}{v},$$

and

$$p_r(v) = -\frac{dh_s}{dv} - \rho_r(v) h_s(v) = \rho_1 \left(1 - \frac{v_1}{v}\right) \exp(-\rho_1 v) + \rho_2 \left(1 - \frac{v_2}{v}\right) \exp(-\rho_2 v),$$

where

$$v_m = \frac{\omega}{\rho_m} \quad m=1,2.$$

The JWL equation of state can be written

$$p(v, e) = \rho_1 \left(1 - \frac{v_1}{v}\right) \exp(-\rho_1 v) + \rho_2 \left(1 - \frac{v_2}{v}\right) \exp(-\rho_2 v) + \frac{\omega}{v} e.$$

A-9.2 Isentrope. The general isentrope has the same form as the Chapman-Jouget isentrope:

$$e_s(v; v_k, e_k) = h_s(v) + \frac{e_k - h_s(v_k)}{(v/v_k)^\omega},$$

or

$$p_s(v; v_k, e_k) = -\frac{dh_s}{dv} + \frac{\omega}{v} \frac{e_k - h_s(v_k)}{(v/v_k)^\omega}.$$

A-9.3 Sound-Speed Functions. Noting that

$$\frac{dp_r}{dv} = \rho_1 \left[\frac{v_1}{v^2} - \rho_1 \left(1 - \frac{v_1}{v}\right) \right] \exp(-\rho_1 v) + \rho_2 \left[\frac{v_2}{v^2} - \rho_2 \left(1 - \frac{v_2}{v}\right) \right] \exp(-\rho_2 v),$$

we can obtain an expression for the square of the sound speed:

$$c^2(v, e) =$$

$$\omega(\omega+1) \left[e_1 \left(\frac{(\rho_1 v)^2}{\omega(\omega+1)} - 1 \right) \exp(-\rho_1 v) + e_2 \left(\frac{(\rho_2 v)^2}{\omega(\omega+1)} - 1 \right) \exp(-\rho_2 v) + e \right].$$

The square of the acoustic impedance and the adiabatic exponent may then be determined from their definitions.

A-9.4 Complete Equation of State. The temperature may be written

$$T = \frac{[p - p_S(v; v_\infty, e_\infty)] v}{\omega c_{vo}} = \frac{e - e_S(v; v_\infty, e_\infty)}{c_{vo}},$$

where v_∞ and e_∞ are determined with reference to a known temperature. The integrating factor for the isentrope pressure is

$$v_S(v) = \frac{f_S(v)}{\rho_T(v)} = \frac{v}{\omega} (v/v_0)^\omega.$$

Thus, the specific entropy is

$$s(p, v) = c_{vo} \log \left(\frac{[p - p_S(v; v_\infty, e_\infty)] v (v/v_0)^\omega}{\omega^2 c_{vo} T_0} \right) = c_{vo} \log \left(\frac{[p - p_S(v; v_\infty, e_\infty)] v^{\omega+1}}{[\rho_0 - p_S(v_0; v_\infty, e_\infty)] v_0^{\omega+1}} \right)$$

or

$$s(v, e) = c_{vo} \log \left(\frac{v^\omega [e - e_S(v; v_\infty, e_\infty)]}{v_0^\omega [e_0 - e_S(v_0; v_\infty, e_\infty)]} \right),$$

where

$$e_o = RT_o + e_s(v_o; v_\infty, e_\infty)$$

and

$$p_o = p_r(v_o) + \omega \frac{e_o}{v_o} ,$$

and the complete equation of state is

$$e(v, s) = RT_o \left(\frac{v_o}{v} \right)^\omega \exp \left(\frac{s}{c_{vo}} \right) + e_s(v; v_\infty, e_\infty) .$$

A-9.5 Hugoniot. The Hugoniot pressure is given by

$$p_H(v; p_u, v_u) = \frac{2[p_r(v) + p_r(v) e_u]v + \omega {}^u\Delta v}{2v - \omega {}^u\Delta v} ,$$

and the minimum specific volume is

$$v_{min} = \frac{\omega}{\omega + 2} v_u .$$

A-10. A JWL Alternative

A-10.1 Incomplete Equation of State for Pressure. An equation of state with a constant Γ is typical of gases. Although Lee and Tarver (1980) have used this form of the JWL equation of state to represent solid materials, they often exhibit behavior consistent with a proportional Grüneisen function:

$$\rho_{\Gamma}(v) = \frac{\Gamma(v)}{v} = \rho_{\Gamma_0} \equiv \frac{1}{v_{\Gamma_0}} ,$$

where ρ_{Γ_0} is a constant. An alternative form of the JWL equation of state reflecting this behavior may be obtained from an isentrope in the form,

$$e_S(v; v_r, e_r) = h_S(v) + \frac{e_r - h_S(v_r)}{\exp[\rho_{\Gamma_0}(v - v_r)]} ,$$

so that

$$p_S(v; v_r, e_r) = -\frac{dh_S}{dv} + \frac{\rho_{\Gamma_0} [e_r - h_S(v_r)]}{\exp[\rho_{\Gamma_0}(v - v_r)]} ,$$

where $h_S(v)$ remains as in the constant- Γ JWL formulation and (v_r, e_r) represents the state defining the reference isentrope. In this case,

$$f_S(v) = \exp[\rho_{\Gamma_0}(v - v_0)] .$$

Thus,

$$\rho_{\Gamma}(v) = \rho_{\Gamma_0} ,$$

and

$$p_{\Gamma}(v) = e_1(\rho_1 - \rho_{\Gamma_0})\exp(-\rho_1 v) + e_2(\rho_2 - \rho_{\Gamma_0})\exp(-\rho_2 v) .$$

The equation of state is

$$p(v, e) = e_1(\rho_1 - \rho_{\Gamma_0})\exp(-\rho_1 v) + e_2(\rho_2 - \rho_{\Gamma_0})\exp(-\rho_2 v) + \rho_{\Gamma_0} e .$$

A-10.2 Isentrope. The isentrope through the state (v_k, e_k) is

$$e_S(v; v_k, e_k) = h_S(v) + \frac{e_k - h_S(v_k)}{\exp[\rho_{\Gamma_0}(v - v_k)]},$$

or

$$p_S(v; v_k, e_k) = -\frac{dh_S}{dv} + \frac{\rho_{\Gamma_0}[e_k - h_S(v_k)]}{\exp[\rho_{\Gamma_0}(v - v_k)]}.$$

A-10.3 Sound-Speed Functions. With

$$\frac{dp_{\Gamma}}{dv} = p_1(\rho_{\Gamma_0} - \rho_1)\exp(-\rho_1 v) + p_2(\rho_{\Gamma_0} - \rho_2)\exp(-\rho_2 v),$$

the square of the acoustic impedance is

$$i^2(v, e) = e_1(\rho_1 - \rho_{\Gamma_0})(\rho_1 + \rho_{\Gamma_0})\exp(-\rho_1 v) + e_2(\rho_2 - \rho_{\Gamma_0})(\rho_2 + \rho_{\Gamma_0})\exp(-\rho_2 v) + \rho_{\Gamma_0}^2 e.$$

The square of the sound speed and the adiabatic exponent may then be determined from their definitions.

A-10.4 Complete Equation of State. The temperature may be written

$$T = \frac{[p - p_S(v; v_{\infty}, e_{\infty})]}{\rho_{\Gamma_0} c_{v0}} = \frac{e - e_S(v; v_{\infty}, e_{\infty})}{c_{v0}},$$

where v_∞ and e_∞ are determined with reference to a known temperature. For a proportional Grüneisen function, the isentrope pressure integrating factor is

$$v_S(v) = \frac{f_S(v)}{\rho_v(v)} = \frac{\exp[\rho_{\Gamma_0}(v-v_0)]}{\rho_{\Gamma_0}},$$

and the specific entropy is

$$\begin{aligned} s(p, v) &= c_{vo} \log \left(\frac{[p - p_S(v; v_\infty, e_\infty)] \exp[\rho_{\Gamma_0}(v-v_0)]}{\rho_{\Gamma_0} R T_0} \right) \\ &= c_{vo} \log \left(\frac{[p - p_S(v; v_\infty, e_\infty)] \exp(\rho_{\Gamma_0} v)}{[\rho_0 - p_S(v_0; v_\infty, e_\infty)] \exp(\rho_{\Gamma_0} v_0)} \right) \end{aligned}$$

or

$$s(v, e) = c_{vo} \log \left(\frac{[e - e_S(v; v_\infty, e_\infty)] \exp(\rho_{\Gamma_0} v)}{[e_0 - e_S(v_0; v_\infty, e_\infty)] \exp(\rho_{\Gamma_0} v_0)} \right),$$

where

$$e_0 = R T_0 + e_S(v_0; v_\infty, e_\infty)$$

and

$$p_0 = p_\Gamma(v_0) + \rho_{\Gamma_0} e_0,$$

and the complete equation of state is

$$e(v, s) = R T_0 \exp \left(\frac{s}{c_{vo}} - \frac{v}{v_{\Gamma_0}} \right) + e_S(v; v_\infty, e_\infty).$$

The Hugoniot pressure is given by

$$\Delta^u p_H(v) = \frac{\Delta^u p_r(v) + \rho_{r_0} (\rho_u^u \Delta v + e_u)}{1 - \frac{1}{2} \rho_{r_0}^u \Delta v},$$

and the minimum specific volume is

$$v_{\min} = v_u - 2 v_{r_0}.$$

Measurement of a solid isentrope for the purpose of calibrating these equations, however, presents some difficulty. The equation is easier to calibrate with reference to Hugoniot data. This is facilitated by converting the measured shock and particle velocities to pressures and specific volumes using the expressions

$$\Delta^a p = \frac{U \Delta^a u}{v_a}$$

and

$$^a \Delta v = \frac{\Delta^a u}{U} v_a.$$

The Hugoniot expression may then be fit to this data in order to obtain values for ρ_1 , ρ_2 , ρ_1 , and ρ_2 . The Grüneisen constant, ρ_r , may also be included in the fit or may be considered known from other sources. In general, this procedure does not provide good fits to linear Hugoniots.

A-11. Hugoniot Equations of State

A-11.1 Hugoniot Reference Functions. The ideal gas and JWL equations of state have been shown to have the general form of the Mie-Grüneisen equation of state. However, the latter is most closely associated with the use of a shock Hugoniot as a reference. An experimentally determined Hugoniot can be used as the basis for developing an equation of state. Generally, however, p - v

measurements are not made. Rather, shock and particle velocities are measured in impact experiments and a curve fit in the form

$$U = U_H(\Delta^a u),$$

is generated for use in lieu of the energy equation. Here, ambient conditions, denoted by the subscript a , give the upstream state. The limit of the shock speed as the upstream state is approached is equal to the ambient sound speed, c_a . Thus,

$$U_H(0) = c_a.$$

In order to be of practical use, the Hugoniot must be expressed in terms of pressure and specific volume, making use of conservation of mass and momentum. Substituting into the momentum equation gives

$$U_H \left(\sqrt{\Delta^a p_H(v; p_a, v_a)} \right) = v_a \sqrt{\frac{\Delta^a p_H(v; p_a, v_a)}{^a \Delta v}}.$$

The functional form of $U_H(\Delta^a u)$ must be chosen such that this equation can be solved for $\Delta^a p_H(v; p_a, v_a)$. A problem arises in generalizing the equation of state to arbitrary upstream states when the experimental Hugoniot is used since it is not clear to what extent $U_H(\Delta^a u)$ depends on the upstream state beyond its known limiting value.

For example, the simplest form of the reference Hugoniot is associated with a linear fit of shock velocity as a function of particle velocity using data for material shocked from the ambient state:

$$U = c_a + s_a \Delta^a u.$$

Many solid materials conform closely to this behavior. The consequent Hugoniot pressure and energy jumps are

$$\Delta^a p_H(v; p_a, v_a) = \frac{c_a^2 {}^a \Delta v}{(v_a - s_a {}^a \Delta v)^2}$$

and

$$\Delta^a e_H(v; p_a, v_a) = \left(p_a + \frac{c_a^2 v_a \Delta v}{2(v_a - s_a^a \Delta v)^2} \right) \Delta v .$$

Note that the reference Hugoniot (and the consequent equation of state) are singular at

$$v = v_{MIN} = \frac{s_a - 1}{s_a} v_a .$$

This singularity arises out of the reference function choice and is distinct from the singularity in the general Hugoniot associated with the Grüneisen function, which occurs at $v = v_{min}$. It limits the utility of the linear Hugoniot equation of state to $v > v_{MIN}$, even though the material it describes can be compressed to smaller volumes by isentropic processes.

The isentrope and sound-speed function expressions make reference to the derivatives of the Hugoniot functions. These are

$$\frac{dp_H}{dv} = - \frac{c_a^2 (v_a + s_a^a \Delta v)}{(v_a - s_a^a \Delta v)^3} = - \frac{v_a + s_a^a \Delta v}{v_a - s_a^a \Delta v} \frac{\Delta^a p_H}{\Delta v} ,$$

and

$$\frac{de_H}{dv} = - p_a - \frac{c_a^2 v_a \Delta v}{(v_a - s_a^a \Delta v)^3} = - \frac{\Delta^a e_H}{\Delta v} - \frac{1}{2} \frac{v_a + s_a^a \Delta v}{v_a - s_a^a \Delta v} \Delta^a p_H .$$

A-11.2 Incomplete Equation of State for Pressure. The equation of state with reference to the ambient Hugoniot can be written

$$p(v, e; p_a, v_a) = p_H(v; p_a, v_a) + \frac{\Gamma(v)}{v} [e - e_H(v; p_a, v_a)] ,$$

or, substituting for the Hugoniot energy from the Hugoniot relation,

$$p(v, e; p_a, v_a) = f_H(v; v_a) p_H(v; p_a, v_a) + \frac{\Gamma(v)}{v} (e - e_a - \frac{1}{2} p_a^a \Delta v) .$$

In writing these equations, we have emphasized the dependence on the choice of an upstream state. The ambient state is commonly used and is a good choice for describing a material that has been shocked from that state. More generally, materials may be multiply shocked and the Hugoniot reference for the most recent upstream state should be more accurate. However, because of the way Hugoniot are measured, such generality is seldom achieved.

The function, $p_\Gamma(v)$, is given by

$$p_\Gamma(v; p_a, v_a) = p_H(v; p_a, v_a) - \rho_\Gamma(v) e_H(v; p_a, v_a) ,$$

or, eliminating the Hugoniot energy,

$$p_\Gamma(v; p_a, v_a) = f_H(v; v_a) p_H(v; p_a, v_a) - \rho_\Gamma(v) (e_a + \frac{1}{2} p_a^a \Delta v) .$$

Differentiating gives

$$\frac{dp_\Gamma}{dv} = \frac{dp_H}{dv} - \rho_\Gamma(v) \frac{de_H}{dv} - e_H(v; p_a, v_a) \frac{d\rho_\Gamma}{dv} ,$$

or

$$\frac{dp_\Gamma}{dv} = f_H(v; v_a) \frac{dp_H}{dv} + \frac{1}{2} \rho_\Gamma(v) [p_a + p_H(v; p_a, v_a)] - e_H(v; p_a, v_a) \frac{d\rho_\Gamma}{dv} .$$

A-11.3 Isentrope. Recalling the relationship between the isentrope and reference energy functions, and using the differentiated Hugoniot relation, we may write

$$e_S(v; v_k, e_k; p_a, v_a) =$$

$$e_H(v; p_a, v_a) + \frac{g_H(v; p_a, v_a) - g_H(v_k; p_a, v_a) + f_S(v_k)[e_k - e_H(v_k; p_a, v_a)]}{f_S(v)},$$

where

$$g_H(v; p_a, v_a) - g_H(v_k; p_a, v_a) = -\frac{1}{2} \int_{v_k} f_S(v) \left(\Delta^a p_H(v; p_a, v_a) + \frac{dp_H}{dv} \Delta v \right) dv.$$

In general, the integral must be evaluated numerically. Forest (1995) has given a method to facilitate the integration. A principal disadvantage of the linear Hugoniot is the absence of analytic expressions for the isentrope internal energy and pressure.

A-11.4 Sound-Speed Functions and Complete Equation of State. The sound speed functions, temperature, and complete equation of state are determined by substitution into the appropriate general equations. No special insight is afforded by this exercise.

A-11.5 Hugoniot. The pressure on a Hugoniot with arbitrary upstream conditions, denoted by the subscript u , is given by

$$p_H(v; p_a, v_a; p_u, v_u) =$$

$$\frac{1}{f_H(v; v_u)} \{ f_H(v; v_a) p_H(v; p_a, v_a) - [1 - f_H(v; v_a)] p_a + [1 - f_H(v; v_u)] p_u + p_T(v) (e_u - e_a) \}.$$

This Hugoniot is valid for

$$v_{MIN} < v_{min} ,$$

where v_{min} depends on the form of the Grüneisen function.

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Appendix B:
Mixture Equations and Derivatives

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B-1. Equations

The equations required to treat mixtures in mechanical and thermal equilibrium are as follows:

Conservation Equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 ,$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p = 0 ,$$

$$\frac{\partial}{\partial t} (\rho e_T) + \nabla \cdot (\rho e_T \mathbf{u}) + \nabla \cdot (p \mathbf{u}) = 0 ,$$

$$e_T = e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} ,$$

$$\frac{\partial}{\partial t} (\rho \lambda) + \nabla \cdot (\rho \lambda \mathbf{u}) = \rho \dot{\lambda}(\lambda, p, \dots) .$$

Mixture Equations:

$$v = (1 - \lambda) v_r + \lambda v_p ,$$

$$e = (1 - \lambda) e_r + \lambda e_p ,$$

$$p = p_r(v_r, e_r + \Delta h_D) ,$$

$$p = p_p(v_p, e_p) ,$$

$$T = T_r(v_r, e_r + \Delta h_D) ,$$

$$T = T_p(v_p, e_p) .$$

The equations required to treat mixtures in mechanical equilibrium and thermal isolation are as follows:

Conservation Equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 ,$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p = 0 ,$$

$$\frac{\partial}{\partial t} (\rho e_T) + \nabla \cdot (\rho e_T \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}) = 0 ,$$

$$e_T = e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} ,$$

$$\frac{\partial}{\partial t} (\rho \lambda) + \nabla \cdot (\rho \lambda \mathbf{u}) = \rho \dot{\lambda}(\lambda, p, \dots) ,$$

$$\frac{\partial}{\partial t} (\rho v_{rk}) + \nabla \cdot (\rho v_{rk} \mathbf{u}) = 0 ,$$

$$\frac{\partial}{\partial t} (\rho e_{rk}) + \nabla \cdot (\rho e_{rk} \mathbf{u}) = 0 .$$

Mixture Equations:

$$v = (1 - \lambda) v_r + \lambda v_p ,$$

$$e = (1 - \lambda) e_r + \lambda e_p ,$$

$$p = p_r(v_r, e_r + \Delta h_D) ,$$

$$p = p_p(v_p, e_p) ,$$

$$p = p_{Sr}(v_r; v_{rk}, e_{rk} + \Delta h_D) .$$

In neither case is closed-form solution of the mixture equations possible. It is necessary to solve the equations using an iterative approach (e.g., Newton's method).

B-2. Derivatives

In order to determine many thermodynamic functions of the mixture, derivatives of the dependent state variables with respect to v , e , and λ are required. A general expression for the differentiated mixture equations that applies to both thermal equilibrium and thermal isolation is given by

$$\begin{bmatrix} 1-\lambda & 0 & \lambda & 0 \\ 0 & 1-\lambda & 0 & \lambda \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \cdot \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ 0 \\ 0 \end{bmatrix}.$$

Here, the a_{3j} and a_{4j} coefficients differ depending on the model. For thermal equilibrium, they are

$$a_{3j} = \left[\left(\frac{\partial p_r}{\partial v_r} \right)_{e_r} \quad \left(\frac{\partial p_r}{\partial e_r} \right)_{v_r} \quad - \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} \quad - \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right],$$

and

$$a_{4j} = \left[\left(\frac{\partial T_r}{\partial v_r} \right)_{e_r} \quad \left(\frac{\partial T_r}{\partial e_r} \right)_{v_r} \quad - \left(\frac{\partial T_p}{\partial v_p} \right)_{e_p} \quad - \left(\frac{\partial T_p}{\partial e_p} \right)_{v_p} \right].$$

For thermal isolation, they are

$$a_{3j} = \begin{bmatrix} -i_r^2 & 0 & -\left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} & -\left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} \end{bmatrix},$$

and

$$a_{4j} = \begin{bmatrix} p & 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} p_r & 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} p_p & 1 & 0 & 0 \end{bmatrix},$$

where the square of the acoustic impedance is

$$i_r^2 = i_{Sr}^2(v_r; v_{rk}, e_{rk}) = -\frac{dp_{Sr}}{dv_r}.$$

The derivative vector, b_i , and the constant vector, c_i , differ depending on whether derivatives are taken with respect to v , e , or λ . For derivatives with respect to v , they are

$$b_i = \begin{bmatrix} \left(\frac{\partial v_r}{\partial v}\right)_{e,\lambda} & \left(\frac{\partial e_r}{\partial v}\right)_{e,\lambda} & \left(\frac{\partial v_p}{\partial v}\right)_{e,\lambda} & \left(\frac{\partial e_p}{\partial v}\right)_{e,\lambda} \end{bmatrix}$$

and

$$c_i = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}.$$

For derivatives with respect to e , they are

$$x_i = \begin{bmatrix} \left(\frac{\partial v_r}{\partial e}\right)_{v,\lambda} & \left(\frac{\partial e_r}{\partial e}\right)_{v,\lambda} & \left(\frac{\partial v_p}{\partial e}\right)_{v,\lambda} & \left(\frac{\partial e_p}{\partial e}\right)_{v,\lambda} \end{bmatrix}$$

and

$$c_i = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}.$$

For derivatives with respect to λ , they are

$$b_i = \left[\left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e} \quad \left(\frac{\partial e_r}{\partial \lambda} \right)_{v,e} \quad \left(\frac{\partial v_p}{\partial \lambda} \right)_{v,e} \quad \left(\frac{\partial e_p}{\partial \lambda} \right)_{v,e} \right]$$

and

$$c_i = \begin{bmatrix} v_r - v_p & e_r - e_p & 0 & 0 \end{bmatrix}.$$

The determinant of coefficients, then, is

$$D = (1-\lambda) [(1-\lambda) A_{34} + \lambda A_{23}] + \lambda [(1-\lambda) A_{41} + \lambda A_{12}],$$

where

$$A_{ij} = \begin{vmatrix} a_{3i} & a_{3j} \\ a_{4i} & a_{4j} \end{vmatrix} = a_{3i} a_{4j} - a_{3j} a_{4i}.$$

Solving for derivatives with respect to v gives

$$\left(\frac{\partial v_r}{\partial v} \right)_{e,\lambda} = \frac{(1-\lambda) A_{34} + \lambda A_{23}}{D},$$

$$\left(\frac{\partial e_r}{\partial v} \right)_{e,\lambda} = \frac{\lambda A_{31}}{D},$$

$$\left(\frac{\partial v_p}{\partial v} \right)_{e,\lambda} = \frac{(1-\lambda) A_{41} + \lambda A_{12}}{D},$$

$$\left(\frac{\partial e_p}{\partial v} \right)_{e,\lambda} = \frac{(1-\lambda) A_{13}}{D},$$

and

$$\begin{aligned}\left(\frac{\partial p}{\partial v}\right)_{e,\lambda} &= \left(\frac{\partial p_r}{\partial v_r}\right)_{e_r} \left(\frac{\partial v_r}{\partial v}\right)_{e,\lambda} + \left(\frac{\partial p_r}{\partial e_r}\right)_{v_r} \left(\frac{\partial e_r}{\partial v}\right)_{e,\lambda} \\ &= \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} \left(\frac{\partial v_p}{\partial v}\right)_{e,\lambda} + \left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} \left(\frac{\partial e_p}{\partial v}\right)_{e,\lambda}.\end{aligned}$$

Similarly, solving for derivatives with respect to e gives

$$\begin{aligned}\left(\frac{\partial v_r}{\partial e}\right)_{v,\lambda} &= \frac{\lambda A_{24}}{D}, \\ \left(\frac{\partial e_r}{\partial e}\right)_{v,\lambda} &= \frac{(1-\lambda) A_{34} + \lambda A_{41}}{D}, \\ \left(\frac{\partial v_p}{\partial e}\right)_{v,\lambda} &= \frac{(1-\lambda) A_{42}}{D}, \\ \left(\frac{\partial e_p}{\partial e}\right)_{v,\lambda} &= \frac{(1-\lambda) A_{23} + \lambda A_{12}}{D},\end{aligned}$$

and

$$\begin{aligned}\left(\frac{\partial p}{\partial e}\right)_{v,\lambda} &= \left(\frac{\partial p_r}{\partial v_r}\right)_{e_r} \left(\frac{\partial v_r}{\partial e}\right)_{v,\lambda} + \left(\frac{\partial p_r}{\partial e_r}\right)_{v_r} \left(\frac{\partial e_r}{\partial e}\right)_{v,\lambda} \\ &= \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} \left(\frac{\partial v_p}{\partial e}\right)_{v,\lambda} + \left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} \left(\frac{\partial e_p}{\partial e}\right)_{v,\lambda}.\end{aligned}$$

Derivatives with respect to λ are given by

$$\begin{aligned}\left(\frac{\partial v_r}{\partial \lambda}\right)_{v,e} &= \frac{(v_r - v_p)[(1-\lambda)A_{34} + \lambda A_{23}] + (e_r - e_p)\lambda A_{24}}{D}, \\ \left(\frac{\partial e_r}{\partial \lambda}\right)_{v,e} &= \frac{(v_r - v_p)\lambda A_{31} + (e_r - e_p)[(1-\lambda)A_{34} + \lambda A_{41}]}{D}, \\ \left(\frac{\partial v_p}{\partial \lambda}\right)_{v,e} &= \frac{(v_r - v_p)[(1-\lambda)A_{41} + \lambda A_{12}] + (e_r - e_p)(1-\lambda)A_{42}}{D}, \\ \left(\frac{\partial e_p}{\partial \lambda}\right)_{v,e} &= \frac{(v_r - v_p)(1-\lambda)A_{13} + (e_r - e_p)[(1-\lambda)A_{23} + \lambda A_{12}]}{D},\end{aligned}$$

and

$$\begin{aligned}\left(\frac{\partial p}{\partial \lambda}\right)_{v,e} &= \left(\frac{\partial p_r}{\partial v_r}\right)_{e_r} \left(\frac{\partial v_r}{\partial \lambda}\right)_{v,e} + \left(\frac{\partial p_r}{\partial e_r}\right)_{v_r} \left(\frac{\partial e_r}{\partial \lambda}\right)_{v,e} \\ &= \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} \left(\frac{\partial v_p}{\partial \lambda}\right)_{v,e} + \left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} \left(\frac{\partial e_p}{\partial \lambda}\right)_{v,e}.\end{aligned}$$

Considerable simplification occurs in the case of thermal isolation, where

$$A_{34} = a_{33} a_{44} - a_{34} a_{43} = 0,$$

$$A_{23} = a_{32} a_{43} - a_{33} a_{42} = \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p},$$

$$A_{41} = a_{34} a_{41} - a_{31} a_{44} = -p_p \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p},$$

$$A_{12} = a_{31} a_{42} - a_{32} a_{41} = -i_r^2,$$

$$A_{24} = -A_{42} = a_{32} a_{44} - a_{34} a_{42} = \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p},$$

and

$$A_{13} = -A_{31} = a_{31} a_{43} - a_{33} a_{41} = p_p \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p}.$$

The determinant of coefficients becomes

$$D_I = \lambda \left\{ -\lambda i_r^2 + (1-\lambda) \left[\left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} - p_p \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right] \right\} = -\lambda [\lambda i_r^2 + (1-\lambda) i_p^2] = -\lambda I^2.$$

Derivatives with respect to v , then, are

$$\begin{aligned}\left(\frac{\partial v_r}{\partial v}\right)_{e,\lambda} &= \frac{-1}{I^2} \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p}, \\ \left(\frac{\partial e_r}{\partial v}\right)_{e,\lambda} &= \frac{p_p}{I^2} \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} = -p_r \left(\frac{\partial v_r}{\partial v}\right)_{e,\lambda}, \\ \left(\frac{\partial v_p}{\partial v}\right)_{e,\lambda} &= \frac{(1-\lambda)p_p}{\lambda I^2} \left(\frac{\partial p_p}{\partial e_p}\right)_{v_p} + \frac{i_r^2}{I^2}, \\ \left(\frac{\partial e_p}{\partial v}\right)_{e,\lambda} &= \frac{-(1-\lambda)p_p}{\lambda I^2} \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p},\end{aligned}$$

and

$$\left(\frac{\partial p}{\partial v}\right)_{e,\lambda} = \frac{-1}{I^2} \left[\left(\frac{\partial p_r}{\partial v_r}\right)_{e_r} - p_r \left(\frac{\partial p_r}{\partial e_r}\right)_{v_r} \right] \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p} = \frac{i_r^2}{I^2} \left(\frac{\partial p_p}{\partial v_p}\right)_{e_p}.$$

Derivatives with respect to e are given by

$$\left(\frac{\partial v_r}{\partial e} \right)_{v,\lambda} = \frac{-1}{l^2} \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p},$$

$$\left(\frac{\partial e_r}{\partial e} \right)_{v,\lambda} = \frac{p_p}{l^2} \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} = -p_r \left(\frac{\partial v_r}{\partial e} \right)_{v,\lambda},$$

$$\left(\frac{\partial v_p}{\partial e} \right)_{v,\lambda} = \frac{1-\lambda}{\lambda l^2} \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p},$$

$$\left(\frac{\partial e_p}{\partial e} \right)_{v,\lambda} = -\frac{1-\lambda}{\lambda l^2} \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + \frac{i_r^2}{l^2},$$

and

$$\left(\frac{\partial p}{\partial e} \right)_{v,\lambda} = \frac{-1}{l^2} \left[\left(\frac{\partial p_r}{\partial v_r} \right)_{e_r} - p_r \left(\frac{\partial p_r}{\partial e_r} \right)_{v_r} \right] \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} = \frac{i_r^2}{l^2} \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p}.$$

Finally, derivatives with respect to λ become

$$\left(\frac{\partial e_r}{\partial \lambda} \right)_{v,e} = \frac{p_p}{I^2} \left[(v_r - v_p) \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + (e_r - e_p) \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right] = -p_r \left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e},$$

$$\left(\frac{\partial v_r}{\partial \lambda} \right)_{v,e} = \frac{1}{I^2} \left[(v_p - v_r) \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + (e_p - e_r) \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right],$$

$$\left(\frac{\partial v_p}{\partial \lambda} \right)_{v,e} = \frac{1}{\lambda I^2} \left\{ (v_r - v_p) \left[(1-\lambda) p_p \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} + \lambda i_r^2 \right] + (e_r - e_p) (1-\lambda) \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right\},$$

$$\left(\frac{\partial e_p}{\partial \lambda} \right)_{v,e} = \frac{1}{\lambda I^2} \left\{ (v_p - v_r) (1-\lambda) p_p \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + (e_p - e_r) \left[(1-\lambda) \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + \lambda i_r^2 \right] \right\},$$

and

$$\left(\frac{\partial p}{\partial \lambda} \right)_{v,e} = \frac{1}{I^2} \left[\left(\frac{\partial p_r}{\partial v_r} \right)_{e_r} - p_r \left(\frac{\partial p_r}{\partial e_r} \right)_{v_r} \right] \left[(v_p - v_r) \left(\frac{\partial p_p}{\partial v_p} \right)_{e_p} + (e_p - e_r) \left(\frac{\partial p_p}{\partial e_p} \right)_{v_p} \right].$$

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1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE March 2000		3. REPORT TYPE AND DATES COVERED Oct 97-Sep 99
4. TITLE AND SUBTITLE Dynamics and Thermodynamics of Simple Two-Phase Reacting Mixtures for Application to Explosive Initiation Modeling			5. FUNDING NUMBERS 1L162618AH43	
6. AUTHOR(S) John Starkenberg				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory ATTN: AMSRL-WM-TB Aberdeen Proving Ground, MD 21005-5066			8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-2161	
9. SPONSORING/MONITORING AGENCY NAMES(S) AND ADDRESS(ES)			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) The front-tracking "hydrocode" FronTier limits finite-difference solution of the dynamic continuum mechanics equations to regions bounded by tracked fronts (shock waves, contact discontinuities, and gradient discontinuities) and uses local solutions of the Riemann problem to advance the positions of these fronts. This solution method places stringent requirements on the availability of thermodynamics information. With the addition of an appropriate reacting mixture model, the code can be applied to solid explosive initiation problems. The required thermodynamic functions are more difficult to obtain for reacting mixtures even though the equations of state for each of the phases present are known. We have developed a mixture model based on assumptions of mechanical equilibrium and thermal isolation that can be used independent of the choice of equations of state for the phases, and we have derived expressions for the necessary thermodynamic functions.				
14. SUBJECT TERMS thermodynamics, explosive initiation modeling			15. NUMBER OF PAGES 95	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

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